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**FISCAL YEAR 2000 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES  
MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY**

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## **PREFACE**

This document summarizes the Fiscal Year 2000 research and operational activities of the Atmospheric Sciences Modeling Division (ASMD), Air Resources Laboratory, working under Interagency Agreements EPA DW13938483 and DW13948634 between the U.S. Environmental Protection Agency (EPA) and the National Oceanic and Atmospheric Administration (NOAA). The summary includes descriptions of research and operational efforts in air pollution meteorology, air pollution control activities, and abatement and compliance programs.

Established in 1955, the Division serves as the vehicle for implementing the agreements with EPA, which funds the research efforts in air pollution meteorology. ASMD conducts research activities in-house and through contract and cooperative agreements for the National Exposure Research Laboratory and other EPA groups. With a staff consisting of NOAA, EPA, and Public Health Service Commissioned Corps personnel, ASMD also provides technical information, observational and forecasting support, and consulting on all meteorological aspects of the air pollution control program to many EPA offices, including the Office of Air Quality Planning and Standards. The primary groups within ASMD are the Atmospheric Model Development Branch, Modeling Systems Analysis Branch, Applied Modeling Research Branch, and Air Policy Support Branch. The staff is listed in Appendix G. Acronyms, publications, and other professional activities are listed in the remaining appendices.

Any inquiry on the research or support activities outlined in this report should be sent to the Director, Atmospheric Sciences Modeling Division (MD-80), Environmental Protection Agency, Research Triangle Park, NC 27711.



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# **FISCAL YEAR 2000 SUMMARY REPORT OF THE NOAA ATMOSPHERIC SCIENCES MODELING DIVISION TO THE U.S. ENVIRONMENTAL PROTECTION AGENCY**

**ABSTRACT.** During Fiscal Year 2000, the Atmospheric Sciences Modeling Division provided meteorological and modeling assistance to the U.S. Environmental Protection Agency. This ranged from the conduct of research studies and model applications to the provision of advice and guidance. Research efforts emphasized the development and evaluation of air quality models using numerical and physical techniques supported by field studies. Among the significant research studies and results were the distribution of Models-3/CMAQ version 3, continued evaluation and modification of CMAQ, modification of CMAQ for toxic air pollutants, implementation of a new emission processing system, initiation of the modeling of particulate matter and air toxics at neighborhood scales, continuation of the work on the Multimedia Integrated Modeling System, analysis of dry deposition field data and development of the next generation deposition velocity model, SODAR and tower meteorological measurements for use in human exposure modeling, and continued study of the wind erosion of sand.

## **1. INTRODUCTION**

In Fiscal Year 2000, the Atmospheric Sciences Modeling Division (ASMD) continued its commitment for providing goal-oriented, high-quality research and development, and operational support to the U.S. Environmental Protection Agency (EPA). Using an interdisciplinary approach emphasizing integration and close cooperation with EPA and public and private research communities, the Division's primary efforts were studying processes affecting dispersion of atmospheric pollutants, modeling pollutant dispersion on all temporal and spatial scales, and developing multi-media model frameworks in a high computing and communications environment. The technology and research products developed by the Division are transferred to the public and private national and international user communities. Section 2.1 discusses Division participation in international activities, while Sections 2.2 through 2.4 outline the Division research activities in support of the short- and long-term needs of the EPA and environmental community. Section 2.5 discusses Division support to the operational programs and general air quality model user community.

## **2. PROGRAM REVIEW**

### **2.1 Office of the Director**

The Office of the Director provides direction, supervision, program management, and administrative support in performing the Division's mission and in achieving its goals of advancing the state of the atmospheric sciences and enhancing the protection of the environment. The Director's Office also engages in several domestic and international research exchange activities.

#### **2.1.1 NATO Committee on the Challenges of Modern Society**

The North Atlantic Treaty Organization (NATO) Committee on the Challenges of Modern Society (CCMS) was established in 1969 with the mandate to examine how to improve, in every practical way, the exchange of views and experience among the Allied countries in the task of creating a better environment for their societies. The Committee considers specific problems of the human environment with the deliberate objective of stimulating corrective action by member governments. The Committee's work is carried out on a decentralized basis through pilot studies, discussions on environmental issues, and fellowships.

##### **2.1.1.1 International Technical Meetings**

The Division Director serves as the United States representative on the Scientific Committee for International Technical Meetings (ITMs) on Air Pollution Modeling and Its Application, sponsored by NATO/CCMS. A primary activity within the NATO/CCMS Pilot Study on Air Pollution Control Strategies and Impact Modeling is organizing a symposium every eighteen months that deals with various aspects of air pollution dispersion modeling. The meetings are rotated among different NATO and Eastern Bloc countries, with every third ITM held in North America and the two intervening ITMs held in European countries.

The Division Director served as the Conference Chairman of the Millennium (24th) NATO/CCMS International Technical Meeting held in Boulder, Colorado, May 15–19, 2000. The proceedings will be published by Plenum Press as were the proceedings from the 23rd ITM held in Varna, Bulgaria, during September–October 1998 (*Air Pollution Modeling and Its Application XIII*, 2000). A preliminary summary of the Millennium ITM is included in the Newsletter of the European Association for the Science of Air Pollution (Schiermeier, 2000). The NATO/CCMS Scientific Committee selected Louvain-La-Neuve, Belgium, as the site for the 25th International Technical Meeting to be held during October 15–19, 2001.

### **2.1.1.2 Regional/Transboundary Transport of Air Pollution**

The Division Director serves as the United States representative on the International Oversight Committee for the NATO/CCMS Pilot Study on Regional/Transboundary Transport of Air Pollution. The aim of the pilot study, sponsored by Greece and approved by NATO in March 1998, is to improve the exchange of views and experience among participating countries in the field of regional/transboundary transport of air pollution. The initial organizing meeting was held in Varna, Bulgaria, during September 1998 in conjunction with the NATO/CCMS International Technical Meeting. The framework for the pilot study was revised to reflect inputs of the meeting participants.

### **2.1.2 United States/Japan Environmental Agreement**

The Division Director serves as the United States Co-Chairman of the Air Pollution Meteorology Panel under the United States/Japan Agreement on Cooperation in the Field of Environment. The purpose of this 1975 agreement is to facilitate, through mutual visits and reciprocal assignments of personnel, the exchange of scientific and regulatory research results pertaining to control of air pollution. Interactions are maintained through correspondence and exchange of research findings.

### **2.1.3 United States/Russia Joint Environmental Committee**

The Division Director serves as the United States Co-Chairman of the United States/Russia Working Group 02.01-10 on Air Pollution Modeling, Instrumentation, and Measurement Methodology, and as Co-Leader of the United States/Russia Project 02.01-11 on Air Pollution Modeling and Standard Setting. The purpose of the 1972 Nixon-Podgorny Agreement forming the US/USSR Joint Committee on Cooperation in the Field of Environmental Protection was to promote, through mutual visits and reciprocal assignments of personnel, the sharing of scientific and regulatory research results related to the control of air pollution. Activities under this agreement were extended to also comply with the 1993 Gore-Chernomyrdin Agreement forming the United States/Russia Commission on Economic and Technological Cooperation. There are four Projects under Working Group 02.01-10:

- Project 02.01-11: Air Pollution Modeling and Standard Setting
- Project 02.01-12: Instrumentation and Measurement Methodology
- Project 02.01-13: Remote Sensing of Atmospheric Parameters
- Project 02.01-14: Statistical Analysis Methodology and Air Quality  
Trend Assessment

Progress under this Working Group continued during FY-2000. An abbreviated Working Group meeting was held during May 2000 in conjunction with the NATO/CCMS International

Technical Meeting in Boulder, Colorado. Plans were made for a full Working Group meeting to be held during November 2000 at the Main Geophysical Observatory in St. Petersburg, Russia.

#### **2.1.4 Meteorological Coordinating Committees**

##### **2.1.4.1 Federal Meteorological Committee**

The Division Director serves as the Agency representative on the Federal Committee for Meteorological Services and Supporting Research (FCMSSR). The Committee is composed of representatives from 14 Federal government agencies and is chaired by the Under Secretary of Commerce for Oceans and Atmosphere, who is also the NOAA Administrator. FCMSSR was established in 1964 with high-level agency representation to provide policy guidance to the Federal Coordinator for Meteorology, and to resolve agency differences that arise during coordination of meteorological activities and the preparation of Federal plans in general.

##### **2.1.4.2 Interdepartmental Meteorological Committee**

The Division Director serves as the Agency representative on the Interdepartmental Committee for Meteorological Services and Supporting Research (ICMSSR). The Committee, composed of representatives from 14 Federal government agencies, was formed in 1964 under Public Law 87-843 and OMB Circular A-62 to provide the Executive Branch and the Congress with a coordinated, multi-agency plan for government meteorological services and for those research and development programs that directly support and improve these services. The Committee prepared the annual *Federal Plan for Meteorological Services and Supporting Research* (U.S. Department of Commerce, 2000).

The Division Director also serves on the ICMSSR Committee for Cooperative Research and on the ICMSSR Joint Action Group for High Performance Computing and Communications. Other Division members serve on the ICMSSR Working Group for Atmospheric Transport and Diffusion and on the ICMSSR Working Group for Climate Services.

#### **2.1.5 Board on Atmospheric Sciences and Climate**

The Division Director serves as the Agency liaison to the Board on Atmospheric Sciences and Climate (BASC) of the National Research Council, National Academy of Sciences. BASC seeks to advance the understanding of the atmosphere and climate, and to improve the ability to apply this knowledge. The Board (1) reviews in broad perspectives both basic and applied research dealing with the atmosphere and with the geophysical systems influencing weather and climate; (2) provides advice and guidance to appropriate government agencies on problems and programs within the Board's interest and expertise; and (3) counsels the United States

participation in such international research and application programs relating to the atmosphere and climate as the World Climate Program and its research activities.

#### **2.1.6 Standing Air Simulation Work Group**

The Division Director serves as the EPA Office of Research and Development representative to the Standing Air Simulation Work Group (SASWG), which serves as a forum for issues relating to air quality simulation modeling of criteria and other air pollutants from point, area, and mobile sources. Its scope encompasses policies, procedures, programs, model development, and model application. The work group fosters a consensus between the Agency and the State and local air pollution control programs through semi-annual meetings of members representing all levels of enforcement.

#### **2.1.7 Trans-Pacific Transport of Atmospheric Contaminants**

The Division Director participated in the First International Conference on Trans-Pacific Transport of Atmospheric Contaminants held in Seattle, Washington, during July 27–29, 2000. The purposes of the conference were to (1) map the state of scientific knowledge on long-range transport of air pollutants into and across the Pacific Ocean from emission sources around the Pacific Rim and beyond; and (2) make recommendations on the next scientific steps needed to clarify uncertainties related to the state of knowledge about trans-Pacific air pollution. This includes identifying data gaps, requirements for integrating present programs, and possibilities for creation of new international cooperative research programs. The Conference Consensus Statement released by the EPA in the form of a press release is available at <http://www.epa.gov/oia/iepi/transpac/htm>. A related article by the conference organizers is in *Science* (Wilkening *et al.*, 2000).

#### **2.1.8 NOAA Air Quality and Environmental Forecasting Modeling**

Division scientists were involved in a series of workshops to develop an initiative for NOAA to improve air quality forecasting and prediction. Air quality forecasting is potentially important for the management of urban and coastal areas, transportation, hazard response, and the conservation of water and air resources. NOAA plans to build its program upon the existing research capabilities and upon forming partnerships with the constituents. ASMD brings to the table its achievements in developing the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Of particular relevance to the air quality forecasting initiative are the Division's research areas of adapting meteorology forecast models to air quality applications, the generation of model-ready source emissions fluxes modulated by meteorological forces, and the integration of gas-phase, aqueous, and aerosol chemistry in a comprehensive chemical-transport modeling system.

### **2.1.9 European Monitoring and Evaluation Program**

A Division scientist serves as the United States representative to the European Monitoring and Evaluation Program (EMEP) that oversees the cooperative program for monitoring and evaluation of the long-range transmission of air pollutants in Europe. The primary goal of EMEP is to use regional air quality models to produce assessments evaluating the influence of one country's emissions on another country's air concentrations or deposition. The emphasis has shifted from acidic deposition to ozone and there are emerging interests in fine particulates and toxic chemicals. The United States and Canadian representatives report on North American activities related to long-range transport. The Division scientist also evaluates European studies of special relevance to the program, providing technical critiques of the EMEP work during formal and informal interactions, and develops and coordinates such programs with EMEP as the modeling studies of the Modeling Synthesizing Center West at the Norwegian Meteorological Institute in Oslo, Norway.

### **2.1.10 Chesapeake Bay Program Air Subcommittee and Chesapeake Bay Program Modeling Subcommittee**

A Division scientist is a member of the Air Subcommittee, a working subcommittee of the Chesapeake Bay Program. Previously this Subcommittee was an advisory group to the Implementation Committee. The subcommittee has responsibility for advice and leadership on issues of atmospheric deposition to the watershed and the Bay, on overseeing application of the Extended Regional Acid Deposition Model (Extended RADM) to link atmospheric deposition with watershed models, and in dealing with the potential role of atmospheric deposition on Bay restoration efforts. The Air Subcommittee also works with other Chesapeake Bay committees to define the top priority air quality scenarios to be simulated by the Extended RADM. The Division scientist is also an ex officio member of the Modeling Subcommittee of the Implementation Committee. This Subcommittee has responsibility for overseeing the application of water quality models and coordinating the linkage of Extended RADM with those models and the interpretation of the findings.

Work in FY-2000 focused on completion of the development of the Extended RADM that incorporates the full dynamics of secondary inorganic fine particle formation to study ammonia deposition. Using the newly developed Extended RADM, National Acid Precipitation Assessment Program (NAPAP) ammonia emissions were adjusted through a primitive model inversion. Subsequently, the operational approach to map the reduced nitrogen range of influence was tested and finalized, and the range of influence for 30 subregions was generated with the Extended RADM. Based on this work the reduced nitrogen airshed for the Chesapeake Bay watershed was defined. It was larger than expected. Future work was also defined that would support the Year 2000 Chesapeake Bay Agreement.

### **2.1.11 Megacity Impact on Regional and Global Environments**

A Division scientist was asked to serve as a member of the External Advisory Panel on the Megacity Impact on Regional And Global Environments (MIRAGE) project at the National Center for Atmospheric Research (NCAR) in Boulder, Colorado. The MIRAGE project is an official NCAR program jointly directed by the NCAR Research Aviation Facility and the Atmospheric Chemistry Division. The advisory panel is composed of 11 scientists from academia and Federal agencies, who are presently involved in urban environmental research. The panel is expected to review the overall program inception, review progress of various studies, and participate in the planning of field experiments. The objective of the project is to study how megacities affect the environment on local, regional, and global scales. The study will be carried out through field study data collection to better understand the physical processes and use of models to help diagnose how human activities in megacities produce their impacts. The initial focus will be on two megacities: Mexico City, Mexico, and Beijing, People's Republic of China. In FY-1999, a proposal to the National Science Foundation (NSF) was developed for a first phase umbrella project relating to Mexico City under which universities could send collaborative proposals. Measurement campaigns in Mexico City are envisioned for the wet and dry season. In FY-2000, NSF continued to be interested in the project and suggested a delay in the inception of a field study. A new proposal may be drafted, and dates for the field study are uncertain.

### **2.1.12 North American Research Strategy for Tropospheric Ozone**

The North American Research Strategy for Tropospheric Ozone (NARSTO) program was established in FY-1995 to address ozone research and coordinate collaborative research among all North American organizations performing and sponsoring tropospheric ozone studies. Sponsors include the private sector and State, Provincial and Federal governments of the United States, Canada, and Mexico. In March 2000, the NARSTO Associate Management Coordinator position was implemented and a Division scientist assigned. The primary duties associated with this position include support and continued improvement of the NARSTO Quality Systems Science Center (QSSC) and overall program support to the NARSTO Management Coordinator's Office. The NARSTO QSSC was identified as the location of EPA's national archive for the extensive particulate matter (PM) research data resulting from the Supersites Program.

The coordination of NARSTO Federal research activities is facilitated by the Subcommittee on Air Quality Research of the Committee on Environment and Natural Resources within the National Science and Technology Council. Four science teams were established: Analysis and Assessment; Observations; Modeling and Chemistry; and Emissions. A Division scientist serves as the Co-Chair of the Modeling and Chemistry Team. One major goal of NARSTO is to produce an assessment of the state of tropospheric ozone science. A draft report was written and reviewed by the National Academy of Sciences (NAS). The NARSTO Ozone Assessment was published in FY-2000 (NARSTO Synthesis Team, 2000). Approximately three



thousand copies of the report were printed for distribution. The Division scientist was chosen to co-author one of the 24 critical review papers that were commissioned to provide technical background to the NARSTO assessment group. During FY-2000, the critical review paper on modeling and evaluation of advanced models was published (Russell and Dennis, 2000). A total of 17 of the 24 critical review papers were published (*Atmospheric Environment*, 2000).

In FY-1998, the NARSTO Executive Assembly decided to include fine-particle research activities under its purview. During FY-2000, a draft PM Science Research Plan was written by the science team chairs. The draft plan is under review by NAS and priorities for PM research are being developed. The next NARSTO state-of-science assessment will focus on particulate matter pollution and how science can be used to develop and implement effective control policies. A NARSTO PM assessment team was charged with completing the final draft assessment report by January 2002 and NAS will review the report by July 2002. The final NARSTO PM Assessment is scheduled for publication in early 2003. The NARSTO Associate Management Coordinator is an active member of the PM assessment team.

### **2.1.13 International Task Force on Forecasting Environmental Change**

A Division scientist is a member of the International Task Force on Forecasting Environmental Change that addresses the methodological and philosophical problems of forecasting under the expectation of significant structural changes in the behavior of physical, chemical or biological systems. Three planned workshops were held at the International Institute for Applied Systems Analysis in Laxenburg, Austria. Internal reviews were completed, and a draft monograph of the workshop discussions was finished in FY-1999. A publisher for the monograph was found in FY-2000.

### **2.1.14 Regional Acid Deposition Model Application Studies**

During FY-2000 an operational version of the Extended RADM that operates on the Cray® T3D™<sup>1</sup> massively parallel computer was completed for application studies. The Extended RADM incorporates the full dynamics of secondary inorganic fine particle formation to be able to simulate ammonia (reduced nitrogen) deposition in addition to oxidized nitrogen deposition. The full coupling is required to account for ammonia deposition and partitioning of total ammonia into gaseous ammonia and particulate ammonium. Ammonia deposition is a major new focus of assessment for deposition to the Chesapeake Bay watershed and Bay surface waters, and to the Neuse River Estuary and Pamlico Sound of North Carolina. The new model will allow the extension of the estimation of airsheds to ammonia. As part of the preparation of the model for applications, the primitive model inversion done with RADM/RPM (Regional Particulate Model) to adjust the NAPAP ammonia emissions to more realistic values was redone

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<sup>1</sup>Cray is a registered trademark and Cray T3D is a trademark of Cray Research.

with the Extended RADM, taking advantage of the full dynamics in the model. The Extended RADM represents a step in the transition to Models-3/CMAQ for application simulations.

In FY-1999, oxidized nitrogen range of influence mapping was completed for more than 100 emission source subregions to support the development of airshed estimates for coastal estuaries. RADM runs for these mappings were completed during FY-1998 and FY-1999, requiring more than 6,000 Cray®-C90<sup>TM2</sup> computer hours. Using the procedure developed for the Chesapeake Bay and outlined in Dennis (1997), airsheds for 19 coastal watersheds along the East and Gulf Coasts were developed. In FY-2000, several airsheds were adjusted and a 20th coastal estuary was added. These oxidized nitrogen airsheds are expected to be available on the Division's multi-media web site in FY-2001. This work is coordinated with the NOAA assessment of atmospheric deposition to coastal estuaries that will be published during the next fiscal year.

In FY-2000, reduced nitrogen range of influence mapping was completed for 45 emission source subregions to support the development of airshed estimates for ammonia. Reduced nitrogen airsheds for Chesapeake Bay and Neuse/Pamlico Sound watersheds were developed. These reduced nitrogen airsheds will be available on the Division's multi-media web site in FY-2001.

#### **2.1.15 International Association of Aquatic and Marine Science Librarians and Information Centers**

The Division Librarian participated in the 25th International Association of Aquatic and Marine Science Libraries and Information Centers (IAMSLIC) Annual Conference, October 16–22, 1999, in Woods Hole, Massachusetts. At the conference, the Librarian presented an informational poster on the membership representation of the Atmospheric Science Librarians International (ASLI) organization. The Librarian worked with the IAMSLIC Vice Chair and Program Planner in selecting topics for the 2001 IAMSLIC Conference to be held in Victoria, British Columbia, Canada, September 28–October 6, 2000, and reviewed and rated abstracts submitted for presentation at the Conference.

#### **2.1.16 Southeast Affiliate of IAMSLIC Librarians**

The Division Librarian hosted the SAIL 2000 Conference during April 2000 in Research Triangle Park, North Carolina. The theme of the SAIL (Southeast Affiliate of IAMSLIC) Conference was *Harness the Power of Information*. Five of the invited speakers were faculty members from the University of North Carolina at Chapel Hill School of Law and the School of Information and Library Science, Chapel Hill, North Carolina. They addressed relevant topics,

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<sup>2</sup>Cray is a registered trademark and Cray C90 is a trademark of Cray Research.

including the digital millennium copyright act, competencies for special librarians, cross-discipline collaboration, marketing library services, and ethics at the virtual reference desk. Two invited scientists gave presentations on the short-term impacts of hurricanes on water quality and fisheries habitat in the Pamlico Sound, and on atmospheric deposition of nutrients to coastal waters of the East and Gulf Coasts. Other presentations were made by SAIL members and publishers and vendors. The 20 regional attendees included NOAA Librarians from the Miami Regional Library, Atlantic Oceanographic and Meteorological Laboratory, the NOS Center for Coastal Fisheries and Habitat Research, and NMFS Panama City Marine Fisheries Laboratory. Additional attendees included librarians and scientists from the academic community, a non-profit laboratory, EPA, and Division staff.

### **2.1.17 Atmospheric Science Librarians International**

The Division Librarian participated in the Third Annual Conference of the Atmospheric Science Librarians International (ASLI), which was held in conjunction with the 80th Annual Meeting of the American Meteorological Society, January 9–14, 2000, in Long Beach, California. The Librarian was elected Chair of ASLI for 2000. As Chair, the Librarian will plan the program for the Fourth Annual Conference, which will be held January 17–19, 2001, in Albuquerque, New Mexico.

### **2.1.18 Atmospheric Sciences Modeling Division Library Home Page**

The ASMD Library maintains a world-wide web (WWW) home page (<http://www.epa.gov/asmdnerl/library/library.htm>), which provides a brief overview of the Library's history and location. The purpose of the home page is to make accessible information about the Library's collection, policies, and services to the Division staff and other users in Research Triangle Park, North Carolina, and other locations. The home page provides WWW interface connections to the EPA and NOAA on-line catalogs in which the Library's book and journal collections are cataloged. In addition, the page provides links to other information resources through the agencies' home pages and to other WWW resources that reflect the Library's collection and staff needs. Division library staff provided HTML (HyperText Markup Language) documents of the FY-1999 annual report and publication citations for inclusion on the Division's home page (<http://www.epa.gov/asmdnerl/>) and publication citations for the NOAA Air Resources Laboratory home page (<http://www.arl.noaa.gov/>).

## **2.2 Atmospheric Model Development Branch**

The Atmospheric Model Development Branch develops, evaluates, and validates analytical and numerical models that describe the transport, dispersion, transformation, and removal/resuspension of atmospheric pollutants on local, urban, and regional scales. These are

comprehensive air quality modeling systems that incorporate state-of-science formulations describing physical and chemical processes.

## **2.2.1 Models-3/Community Multiscale Air Quality Modeling**

### **2.2.1.1 Introduction**

EPA released the Models-3/Community Multiscale Air Quality (CMAQ) modeling system, initially in June 1998, and two subsequent revisions in FY-1999 and FY-2000. Models-3/CMAQ is a numerical modeling system that can simultaneously simulate the transport, physical transformation, and chemical reactions of multiple pollutants across large geographic regions. The system is useful to states and other government agencies for making regulatory decisions on air quality management, as well as to research scientists for performing atmospheric research. It is a combination of Models-3, a flexible software framework, and the CMAQ modeling system for supporting air quality applications ranging from regulatory issues to scientific research on atmospheric processes. A modular science design of CMAQ allows the user to build different chemistry-transport models for various air quality problems. The CMAQ models can be operated independently of the Models-3 system framework, providing more flexibility for advanced research and applications. The CMAQ models were tested for several air quality studies, including photochemical ozone and particular matter episodes in the 1995 northeastern United States (NARSTO-NorthEast field study) and southeastern United States (Nashville, Tennessee, Southern Oxidants Study (SOS)) for the period July 2–18, 1995. The test results are very promising when compared with observed surface ozone concentrations and aircraft measurements. A rigorous evaluation effort is continuing through FY-2001.

In FY-2000, the EPA document, *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System* (U.S. Environmental Protection Agency, 1999), was distributed to many different air quality modeling groups in the United States and around the world. The document's 18 chapters describe all the key state-of-science atmospheric science features and options that are embodied in the CMAQ system. Collectively, it provides the scientific basis and point of reference for the state of the science captured in the June 1999 release of the CMAQ modeling system. The document is available for download at <http://www.epa.gov/asmdnerl/models3/CMAQ/index.html>.

### **2.2.1.2 Research and Development Scope of the Community Multiscale Air Quality Modeling System**

After the initial release of the Models-3/CMAQ system, development continued to improve its science content and expand the operational platforms. The Models-3/CMAQ science paradigm embodies the one-atmosphere concept for air quality modeling. To simulate weather and air quality phenomena realistically, adaptation of a one-atmosphere perspective based mainly on first principle science descriptions of the atmospheric system is necessary. This perspective

emphasizes the interactions among multiple air pollutants at different dynamic scales. For example, processes critical to producing oxidants, acid and nutrient depositions, and fine particles are too closely related to be treated separately. Proper modeling of these air pollutants requires simultaneous consideration of the broad range of temporal and spatial scales of multi-pollutant interactions. Another key aspect of the one-atmosphere perspective is the dynamic description of the atmosphere. Air quality modeling should be viewed as an integral part of atmospheric modeling and the governing equations and computational algorithms should be consistent and compatible.

Science submodels in the CMAQ system are the Mesoscale Model Version 5 (MM5), Models-3 Emissions Processing and Projection System (MEPPS), and the CMAQ Chemical-Transport Model (CCTM). There are several interface processors that link other model input data to CCTM. The Meteorology-Chemistry Interface Processor (MCIP) processes MM5 output to provide a complete set of meteorological data needed for CCTM. Initial and boundary conditions are processed with the processors, ICON and BCON, respectively, and the Emissions-Chemistry Interface Processor (ECIP) combines area- and point-source emissions to generate three-dimensional gridded emission data for CCTM. A photolytic rate constant processor, which is based on RADM's JPROC, computes species-specific photolysis rates for a set of predefined zenith angles and altitudes. An alternative detailed-science version adopts state-of-the-science radiative transfer models with a possibility of taking into account the total ozone column from TOMS satellite data and turbidity. In addition, a Plume Dynamics Model (PDM) is used to provide major elevated point-source plume dispersion characteristics for driving the plume-in-grid processing within CMAQ. The continued improvement of many elements of the CMAQ system is described below.

The third public release of the CMAQ modeling system occurred in July 2000. There were few science changes to CMAQ although significant changes were made in the emissions data and the physics options used with MM5. The FY-2000 CMAQ release was tested against data from the 1995 NARSTO-NorthEast field study and 1995 Nashville, Tennessee, SOS field experiment. This version of the model is configured for use by the EPA Office of Air Quality Planning and Standards (OAQPS) and other groups involved in policy and regulatory analyses for air quality management. CMAQ was configured with the Carbon Bond-IV (CB-IV) chemical mechanism for these tests, the same mechanism used in other ozone air quality models for regulatory purposes. Model testing will continue in FY-2001, and will include examining the impacts of decreasing the vertical resolution on simulation results.

### **2.2.1.3 Transport Processes within the Community Multiscale Air Quality Modeling System**

CMAQ's modular design promotes incorporation of several sets of science process modules representing different algorithms and parameterizations of physical and chemical processes. For example, there are several different atmospheric transport algorithms and chemistry solvers available within CMAQ. One objective of the study is to demonstrate benefit

of the modularity of the CMAQ system. Another is to assess the effects of different transport algorithms and grid resolutions on air quality predictions. In principle, the atmospheric transport processes, except for the sub-grid scale cloud mixing, are divided into advection and diffusion processes. They are further separated both in the horizontal and vertical directions, respectively.

Differences between the 36-km resolution CMAQ runs were studied with two vertical diffusion algorithms, a non-local asymmetric convective model (ACM), and a local eddy diffusion scheme. The results show that CMAQ with ACM produces higher ozone and  $\text{NO}_y$  concentrations. ACM mixes  $\text{NO}_x$  and VOC emissions much more rapidly, thus resulting in more vigorous photochemical reaction. VOC emissions are mostly from surface sources and  $\text{NO}_x$  emissions are from both the surface (mobile and urban sources) and elevated sources. Therefore, VOC emissions injected into the lowest model layer are moved to the upper boundary layer very quickly by the nonlocal scheme, thus changing the relative composition of the nitrogen and VOC compounds in the simulated air. This may be due to the incoherent representation of the ACM mixing algorithm and the emissions in the system. Treatment of isoprene emissions, for example a species that is affected by the surface turbulence fluxes, and the ACM diffusion module, may not be consistent. An improved ACM version to reconcile these differences is being developed.

CMAQ was tested with two advection algorithms, PPM (piecewise parabolic method) and the Bott scheme. PPM is a positive definite and monotonic scheme, while the Bott scheme is a non-monotonic scheme and could generate unwanted local extreme values for such trace species as aerosol number density that have large concentration gradients. Numerical tests with CMAQ revealed that PPM is more robust for multi-pollutant simulations under various meteorological and chemical conditions. Although simulations with gas-phase species alone were satisfactory, the runs with aerosol dynamics with Bott and the ACM modules were not successful. Apparently, a minor problem with CMAQ's Bott module that replaces very small negative values with zero causes inadvertent re-initialization of aerosol number concentrations in certain cells. Analysis results show that the Bott scheme is less diffusive than PPM, and thus maintains peaks of concentrations better.

In addition, CMAQ results were compared for the cases where emissions were injected either in the vertical diffusion module or in the gas-phase chemical reaction module. This modeling construct affects CMAQ results due to the different titration rates of ozone with fresh NO emissions, thus changing the propagation of radicals at different stages of photochemical evolution. The ozone concentrations were lower for the runs with emissions in chemistry than for those with emissions in the vertical diffusion routines. For the species that have short chemical time scales competing with the transport time scales, the concentration differences are substantial depending on where emissions are injected. Further studies are warranted to establish the proper configuration of process modules in Eulerian air quality models with the time-splitting approach and to determine optimal inter-process time steps.

Finally, the sensitivity of CMAQ with respect to the grid resolution was studied. MM5 runs were made with the nonhydrostatic version and Blackadar boundary-layer parameterization for 12- and 4-km grid resolutions (one way nesting). The Grell cumulus cloud scheme and

analysis nudging were applied only to the 12-km grid. For similar meteorological conditions, higher maxima in the 4-km resolution case than in the 12-km resolution case would be expected, since the sources are resolved better and the initial cloud is smeared in a smaller volume. In the simulations, the wind speeds are higher in the 4-km grid, which would tend to lower the concentrations relative to the 12-km grid. Still, in some cases the 4-km grid concentrations are higher than those in the 12-km grid. MM5 is being run at 4 km with an observation nudging technique to improve consistency in meteorology simulations at different resolutions. Further plans are to run the meteorological model at the 1.3-km grid resolution. It might require implementation of relevant parameterizations to include the drag and the heat balance in urban areas.

It was demonstrated that the choice of modules in transport processes interacts with other model processes. Comparison with observations, especially with secondary species such as  $O_3$ , may not be sufficient to allow selection of the best modules. For example, comparison of the first layer ozone concentrations with those from EPA's AIRS database is not sufficient to determine which transport algorithms are superior. Such factors as the representation of emissions inputs, the treatment of plume-in-grid, the use of different chemical mechanisms, the selection of different chemical solvers, and the model grid structure (*i.e.*, vertical and horizontal resolutions and domain size), all contribute to different model results. Establishment of the best configuration of science process modules in a comprehensive AQM requires balanced representations of transport algorithms with other physical and chemical processes.

#### **2.2.1.4 Photolysis Rates**

Photolysis rates for the Models-3/CMAQ are computed using a table-interpolation method (Roselle *et al.*, 1999). A table was prepared of photolysis rates for different times of day, latitudes, and heights. Photolysis rates for individual grid cells of CMAQ were then computed by interpolating values from the table. In FY-2000, development continued in coupling aerosols and gas-phase chemistry to include the effects of aerosols on photolysis rate calculations (Kondragunta *et al.*, 2000). Testing and evaluation will continue in FY-2001.

#### **2.2.1.5 Cloud Dynamics and Aqueous-Phase Chemistry Module**

The cloud module in CMAQ consists of a sub-grid cloud model and a grid-resolved cloud model (Roselle and Binkowski, 1999). The sub-grid cloud model, which is based on the RADMC cloud module (Walcek and Taylor, 1986; Chang *et al.*, 1990; Dennis *et al.*, 1993), simulates convective precipitating and non-precipitating clouds. The grid-resolved cloud model simulates clouds that occupy the entire grid cell and were resolved by the meteorological model. Several changes were made to the cloud module in FY-2000. The cloud model was revised to consider additional aerosol size-distribution parameters, including surface area. Development was started on the Sulfate-Tracking Model, which will track the sources of sulfate (either gas-phase and aqueous-phase production) at any location and at any time. In addition to work on the cloud

module, integration and testing of a new detailed grid-resolved cloud model continued in FY-2000. Evaluation of the CMAQ cloud model will continue in FY-2001.

#### **2.2.1.6 Subgrid Scale Plume-in-Grid Modeling in the CMAQ Modeling System**

The plume-in-grid (PinG) approach contained in the CMAQ modeling system provides a more realistic scientific treatment of the physical and chemical processes affecting pollutant concentrations in isolated, major point-source plumes. In contrast to the traditional Eulerian grid modeling method of instantly diluting point-source emissions into an entire grid-cell volume, the PinG algorithms simulate the gradual growth of subgrid scale plumes and more properly treat the temporal evolution of photochemistry in individual plume cells during the subgrid scale phase. The PinG algorithms were modified for use on different computer platforms and tested in the Models3/CMAQ modeling system. The revised PinG programs were made available in the June 2000 public release of the CMAQ science algorithms. The capabilities of the PinG model and details of its technical formulation are described in Gillani and Godowitch (1999).

The key modeling components, designed to simulate the relevant plume processes at the proper spatial and temporal scales, include a PDM processor and a Lagrangian reactive plume model (PinG module). The PDM processor determines the position and physical dimensions of individual plume sections by simulating plume rise, vertical and horizontal plume growth, and plume transport. The PinG model simulates the relevant plume processes with a moving array of attached cells representing a plume vertical cross-section (Godowitch *et al.*, 1999). PinG is capable of simulating a single plume or multiple point-source plumes from hourly emission releases. The PinG module is fully integrated into the CCTM. PinG is exercised simultaneously with a CCTM simulation and applies grid concentrations as boundary conditions for the plume sections. An important feedback occurs when a plume section reaches grid cell size, since the subgrid plume treatment ceases and plume concentrations are included in the Eulerian grid.

Simulations were performed with the PinG approach applied to a group of major point sources exhibiting a wide range of NO<sub>x</sub> emission rates within a regional modeling domain encompassing the greater Nashville, Tennessee area (Godowitch and Young, 2000). Qualitatively, the PinG results at various downwind distances were encouraging with the modeled plume NO<sub>x</sub> and ozone concentrations exhibiting the same evolutionary pattern found in real-world plume measurements. A quantitative evaluation of the PinG model is underway with modeled concentrations being compared to observed plume data collected by various airborne platforms during the SOS summer 1995 field experiment in the greater Nashville region with results to be reported in FY-2001. An effort to extend the PinG model to treat aerosol species is planned.



### **2.2.1.7 Air Quality Modeling of Particulate Matter and Air Toxics at Neighborhood Scales**

A project is under way to develop and test a methodology linking Eulerian grid-based air quality models to human exposure models as a tool for understanding, assessing, and quantifying the health impacts and risk of airborne particles and air toxics. Mechanisms under investigation for adverse health impacts consist of numerous causal hypotheses, including concentration loading of fine particulate matter and toxic pollutants and their chemical constituents and physical properties. However, the distribution of pollutant concentration fields for different causal pollutants may be highly complex at neighborhood scales. When formulating the linkages, an important property of air quality modeling simulation is to model at a spatial resolution commensurate with the spatial gradients of the air pollutant fields. Fresh sources of pollutants in urban areas introduced into a regional air mass produce significant sub-urban scale and highly complex spatial variability, and mixtures of particulate and toxic pollutant concentration fields, which correspondingly impact human exposure. For many pollutants that are introduced locally, the design requirement to capture the details of concentration variation requires a grid resolution on the scale of neighborhoods. The proof-of concept exercise, demonstrated the bridging of air quality models with exposure modeling by extending the range of the Models-3/CMAQ spatial resolution capability from its regional- (~36 km) and urban-scale (4 km) resolutions to 1.33 km. The CMAQ modeling system incorporates such state-of-science parametric formulations of all the critical science processes as atmospheric transport, deposition, cloud mixing, emissions, gas and aqueous-phase chemical transformation processes, and aerosol dynamics and chemistry that control the temporal and spatial distribution of the air quality fields. Using CMAQ, with its one-atmosphere paradigm, the scope of this prototype study can encompass the range of air quality and exposure model linkages for photochemical oxidants, particulate matter (PM<sub>10</sub> and PM<sub>2.5</sub>) and air toxics.

The initial study applied the CMAQ modeling system at three grid resolutions, 12, 4 and 1.33 km, in the Philadelphia Metropolitan Area to illustrate the utility of linking CMAQ to the EPA Stochastic Human Exposure and Dose Simulations model for estimating population exposure in Philadelphia. Preliminary results show that the meteorological and subsequent pollutant fields of surface layer ozone and PM<sub>2.5</sub> and its constituent species, as well as the distribution of population exposure, are significantly dependent on the scale of the grid resolution. However, the sensitivity to scale dependency varies between the different air quality fields. Efforts to introduce near-source dispersion modeling are underway. Additionally, studies will be conducted to provide a basis for more robust use of air quality models as a bridge to exposure modeling, including extensions toward modeling semi-volatile organic toxic compounds, improved parameterizations of urban canopies, and pollutant exchanges between microenvironments and the larger scale. Methods to extrapolate episodic model results to longer-term exposure time scales and the use of data-assimilation methods that combine monitoring data with model results will need to be explored.

### 2.2.1.8 Aggregation Research for Models-3/CMAQ

In support of studies mandated by the 1990 Clean Air Act Amendments (CAAA), the Models-3/CMAQ model is used by the EPA Program Offices to estimate deposition and air concentrations associated with specified levels of emissions. Assessment studies require CMAQ-based distributional estimates of ozone, acidic deposition, PM<sub>2.5</sub>, as well as visibility, on seasonal- and annual-time frames. Unfortunately, it is not financially feasible to execute CMAQ over such extended time periods. Therefore, in practice, CMAQ must be executed for a finite number of episodes or events, which are selected to represent a variety of meteorological classes. A statistical procedure called aggregation must then be applied to the outputs from CMAQ to derive the required seasonal and annual estimates.

The objective of this research was to develop a new aggregation approach and set of events to support CMAQ-based distributional estimates of fine particles and other air quality parameters over the continental domain. The primary strategy involved categorizing many years of meteorological patterns into a few classes. This represents a very ambitious goal, and not surprisingly the wind vectors assigned to individual clusters varied substantially. Nevertheless, the results suggest that the approach reasonably characterizes flow patterns associated with synoptic-scale patterns and leads to strata that explain variation in extinction coefficient, temperature, and relative humidity (Eder *et al.*, 2000).

Defining seasonally based clusters further improved the ability of the clusters to explain the variation in these parameters, and therefore led to more precise estimates. The final scheme included 20 clusters (five per season), and stratified systematic sampling was used to select a sample of 40 events from the 20 clusters. The approach performed better than simple random sampling; relative efficiencies were 1.18 for extinction coefficient, 3.86 for temperature, and 1.36 for relative humidity. A basic aggregation technique was also illustrated for the selected sample of events, and revealed aggregated estimates of the  $b_{\text{ext}}$  falling generally within  $\pm 10\%$  of the observed mean  $b_{\text{ext}}$  for the period 1984-1992, consistent with independently estimated variability (Cohn *et al.*, 1999; Cohn *et al.*, in press).

Future work will investigate the ability of the aggregation and episode selection scheme to replicate actual  $b_{\text{ext}}$  on finer temporal and spatial scales to accommodate various applications of CMAQ. For instance, will aggregated estimates of  $b_{\text{ext}}$  for an individual year such as 1988 (a meteorologically anomalous year) still fall within  $\pm 10\%$  of the observed mean, or will the estimates deteriorate?

### 2.2.1.9 Collaborative Model Evaluation Studies for Particulate Matter

Three collaborative model evaluation projects are underway based upon utilization of the Models-3/CMAQ system. Through a cooperative agreement, a modeling center has been initiated at the University of Alabama-Huntsville to develop a Models-3/CMAQ capability to serve present and future needs of the SOS community. As part of the functions of this Center for

Models-3/CMAQ, performance evaluation will be conducted for specific episode simulations. The initial model-data intercomparisons will be made for selected case studies using targeted data from aircraft, meteorological observations, and surface chemistry sites from the 1999 SOS-Nashville field experiment. A research collaboration between the Washington University Center for Air Pollution Impacts and Trend Analysis (CAPITA) in St. Louis, Missouri, and ASMD is underway to evaluate the performance of Models-3/CMAQ, and assess the suitability of using visibility as a surrogate for  $PM_{2.5}$  concentrations in the Models-3/CMAQ aggregation technique for producing annual- and long-term averages. Both efforts will be utilizing CAPITA's consolidated database of PM data sets. This project serves to facilitate the use of Models-3/CMAQ by an extended community. This aids in its evaluation and utility to address major and pertinent issues of developing science-based strategic plans for dealing with NAAQS (National Ambient Air Quality Standards) issues, including  $PM_{2.5}$ ,  $PM_{10}$ , and ozone. This research provides and utilizes methods to perform essential scientific evaluation of the performance of CMAQ in modeling fine particles.  $PM_{2.5}$  modeling is needed for performing environmental assessments and implementing the requirements of the  $PM_{2.5}$  State Implementation Plans (SIPS) and Regional Haze Rule (RHR).

The development, implementation, and utilization of Models-3/CMAQ to assess and develop strategic and tactical strategies to deal with existing and emerging pollution issues pertinent to the Class I natural areas in the West is underway through an interagency agreement with the National Park Service (NPS). NPS, in collaboration with the Cooperative Institute for Research in the Atmosphere at the Colorado State University, Fort Collins, Colorado, has begun its implementation of Models-3/CMAQ and will begin to develop and incorporate algorithms for advanced smoke emission processing from fires (prescribed, agricultural, and natural) in Models-3/CMAQ. This project will facilitate the use of Models-3/CMAQ in the West to develop science-based strategic plans for dealing with smoke emission management issues and interstate transport affecting regional haze,  $PM_{2.5}$ ,  $PM_{10}$ , and ozone.

#### **2.2.1.10 A Preliminary Evaluation of Models-3/CMAQ Using Visibility Parameters**

Ambient air concentrations of  $PM_{2.5}$  continue to be a major concern for EPA. High concentrations of fine particles were linked to detrimental health effects (including an increase in mortality) and visibility degradation. Accordingly, the CAAA of 1990 called for an assessment of current and future regulations designed to protect human health and welfare. The most reliable tool for carrying out such assessments are air quality models, which simulate air concentrations and deposition of  $PM_{2.5}$ , and various measures of visibility associated with specified levels of emissions. These simulations can be used by EPA Program Offices and research laboratories to support both regulatory assessment and scientific studies on a myriad of spatial and temporal scales.

This research provides a preliminary evaluation of CMAQ using a visibility parameter called the deciview. The evaluation compares deciview values computed from visibility observations at 174 stations in the eastern half of the United States with those simulated by the

model for the 5-day period, July 11–15, 1995. Visibility was selected for this evaluation for two reasons: it can serve as a surrogate for  $PM_{2.5}$  for which little observational data exist; and it has one of the most spatially and temporally comprehensive observational data sets available.

The evaluation revealed a general agreement between the modeled and observed values, with over two-thirds of the simulated values falling within a factor of two of the observations (Eder *et al.*, in press). The CMAQ simulation also captured the basic spatial and temporal patterns of visibility degradation, including major gradients and maxima/minima. The correlation coefficient between the observed and simulated deciviews for the entire 5-day simulation period was 0.56 and ranged from 0.38 on July 11 to 0.70 on July 13. The model generally underpredicted the visibility degradation by 10 deciviews; however, some of this discrepancy can be attributed to artifacts associated with the observed data. Other potential sources of CMAQ discrepancies, which will be the subject of future research, include possible errors in the emissions inventories, the input meteorological data, and the aerosol model itself.

### **2.2.2 Aerosol Research and Modeling**

The FY-2000 release of CMAQ incorporated the latest version of the aerosol dynamics code. Integrating the new version within the three-dimensional structure of CMAQ required special treatment. In the FY-1999 release, the total aerosol number and species mass concentrations within the Aitken and accumulation modes were the history variables. Number is the zeroth moment of the size distribution, and mass defines the third moment of the distribution when scaled by a standard density. This means that the geometric standard deviation of each of the modes was a fixed value. In the new version, total surface area, which is a constant times the second moment of the distribution, was added as a history variable; thus, the geometric standard deviation is now a variable. However, this new history variable needs to be transported. This requires some careful analysis. In the real atmosphere, particles adjust to their immediate environment while being transported. Hydrophilic particles take up water in response to increasing relative humidity as, for example, in rising air parcels. In a numerical model, it is very difficult to model this adjustment process exactly as it happens in the atmosphere. The most common method is to take a transport step followed by a thermodynamic adjustment step. Because the model results are desired at a time granularity much coarser than the few seconds that the adjustment takes in the atmosphere, it is acceptable to use this common approach. Note that transport by atmospheric motion can be viewed as a mixing process. In an Eulerian model like CMAQ, transport includes advection of material from one grid cell to an adjacent grid cell. Transport also includes turbulent mixing that occurs in the planetary boundary layer (PBL). Both of these processes may be viewed as combining or mixing values from two grid cells, the source and target cells, with the result being placed in the target cell.

When the aerosol module version with the fixed geometric standard deviation was integrated into the CMAQ code, number and mass concentrations were mixed, water content was adjusted, and the size distribution calculated from the moments. When, however, the second moment is included, the situation is more complex. The second moment (surface area) has

specific information about the size distribution. It can represent the surface area of either wet or dry particles. The number concentration is insensitive to the presence of water. The species mass concentration transported in the FY-1999 version did not include water; this was determined at every time step from the thermodynamic calculations. When surface area was introduced, the first CMAQ calculations were done by transporting the surface area for wet particles. The results did not closely resemble real atmospheric size distributions. The geometric standard deviations appeared to be too large. It was determined that vertical diffusion was the major cause. This may be understood as follows. In the well-mixed daytime PBL, potential temperature and water vapor mixing ratio are very nearly constant with height. But, relative humidity increases in a rising air parcel under these circumstances. Thus, particles at higher altitudes will be larger than particles at lower altitudes. Now consider the mixing of the moments of two size distributions, one with a higher water content than the other. If the geometric standard deviations are equal, but the diameters are different, the resultant size distribution will have a larger geometric standard deviation. This was the cause of the problem with the modeled size distributions. If, however, the second moment is for a dry particle size distribution in the well-mixed PBL, the difference in the moments is much smaller, and the resulting size distributions are more realistic. Therefore, all transport is done with the surface area (second moment) being calculated for a dry particle size distribution in the FY-2000 release of CMAQ. After the transport step, but before any aerosol dynamics calculations are done, the distributions are adjusted for humidity. The new wet size distribution is used for all further dynamical and visual range calculations. Before the next transport step, the size distribution is readjusted to be a dry distribution to continue the model simulation.

## **2.2.3 Atmospheric Toxics Pollutant Research**

### **2.2.3.1 Atmospheric Toxics Pollutant Modeling**

During FY-2000, a modeling study was concluded using previously developed simulation capabilities for atmospheric mercury based on the REgional Lagrangian Model of Air Pollution (RELMAP) (Eder *et al.*, 1986) to investigate the incremental effects of mercury air emissions from Canada on the magnitude and pattern of mercury deposition across the United States. Development of new atmospheric simulation modeling capabilities for toxic pollutants during FY-2000 focused on two pollutants: mercury and the semi-volatile pesticide atrazine. Both modeling efforts involve the use of CMAQ as the basis for air toxics pollutant modeling, but their relevant scientific issues and modeling approaches differ somewhat. Each effort is discussed separately below.

#### **Modeling of Mercury.**

The RELMAP mercury model was developed to simulate the emission, transport, dispersion, atmospheric chemistry, and deposition of mercury across the continental United States (Bullock *et al.*, 1997). This model was used in the development of the *Mercury Study Report to Congress* (U.S. Environmental Protection Agency, 1997) to estimate the magnitude

and pattern of mercury deposition throughout the United States from domestic emissions and from the global average concentration of elemental mercury from sources all around the world. During FY-2000, an inventory of Canadian air emissions of mercury was added to the simulation to revise previous mercury deposition estimates. The atmospheric fate of Canadian mercury emissions was simulated in the same manner as previously done for United States emissions, and an assessment of the incremental effect of Canadian sources on the total mercury deposition pattern across the United States was obtained. These results suggest that Canadian sources account for no more than 20 percent of mercury deposition to any U.S. location, with the exception of the extreme northern section of the Rocky Mountain region near the Canadian border. An article describing this modeling exercise and its results was accepted for publication (Bullock, in press).

In FY-2000, a number of gas- and aqueous-phase chemical reactions involving mercury were added to CMAQ. The standard CMAQ gas- and aqueous-phase chemistry mechanisms for tropospheric ozone and acid deposition simulation are used as a basis for the simulation of complex mercury chemistry. During FY-2000, new aqueous-phase reactions of elemental mercury with dissolved chlorine species  $\text{OCl}^-$  and  $\text{HOCl}$ , and dissolved  $\text{OH}$  radical were added to CMAQ. Reactions of all modeled forms of dissolved  $\text{Hg}^{++}$  with  $\text{HO}_2$  radical to form elemental mercury were also added. These new reactions were based on Lin and Pehkonen (1999) and Pehkonen and Lin (1998). A previously included reaction of  $\text{HgSO}_3$  to form elemental mercury by spontaneous decomposition was modified based on the results of a new analysis of the reaction rate (Van Loon *et al.*, 2000). This new information indicates that the production of elemental mercury is much slower than previously thought, and that additional mercury-reducing agents must be important to the overall reduction-oxidation balance of mercury in cloud water and precipitation.

During FY-2000, Branch personnel participated in the first phase of an international atmospheric mercury model intercomparison sponsored by the European Monitoring and Evaluation Programme (EMEP) and organized by EMEP's Meteorological Synthesizing Center - East (MSC-East) in Moscow, Russia. This first phase of the intercomparison involved the simulation of mercury chemistry in a closed cloud volume given a variety of initial conditions. Results obtained from the CMAQ mercury model and the other participating models from Russia, Germany, Sweden, and the United States are now being compared to identify key scientific and modeling uncertainties, and a report will be issued by the MSC-East. In FY-2001, a second phase of intercomparison is planned, which will involve full-scale model simulations of the emission, transport, transformation and deposition of mercury over Europe and comparison of the modeling results to corresponding field measurements.

### **Modeling of Semi-Volatile Compounds.**

To simulate the fate of compounds that are considered semi-volatile and toxic, CMAQ was modified to introduce a semi-volatile compound into the atmosphere as gaseous emissions from an area source. Once emitted, the gas can transform via  $\text{OH}$  addition or partition onto ambient particulate matter as a trace species. The partitioning assumes equilibrium between the

gas and particulate phases based on empirical and theoretical work (Pankow, 1987; 1994). Concentrations in each phase then depend on the total ambient concentration and partitioning ratios. Besides these chemical and physical processes, the compound undergoes advection, diffusion, and deposition.

CMAQ was selected to address this issue based on how the model estimates particulate matter in the lower troposphere. The estimate uses a tri-modal distribution and internal mixture of inorganic and organic species to describe particulate matter. The inorganic species divide into two components: aqueous and dry. These aspects permit studying how a semi-volatile compound partitions onto particulate matter in different ways. The compound adsorbs onto surface areas from a combination of inorganic species within particulate matter. In addition, the semi-volatile compound absorbs into either the organic species or aqueous component within particulate matter. CMAQ then is able to help assess how meteorology and gas-to-particle partitioning combine to control the fate of semi-volatile compounds over regional and local scales.

The modified model is being evaluated through the simulation of atrazine, a common agricultural herbicide. The effort uses atrazine emissions predicated on its usage, and a soil model under energy balance conditions. The model domain covers the eastern United States and the simulation spans the period from April to mid-July of 1995. Results include concentrations in air and precipitation. Baseline calculations are being used to support assessments conducted by the Lake Michigan Mass Balance Study. Comparisons of model results to observations (Majewski *et al.*, 2000; Foreman *et al.*, 2000) show on average that the model underpredicts precipitation concentrations while it overpredicts air concentrations. These findings imply that the model's algorithms insufficiently scavenge airborne atrazine via wet deposition. Sensitivity calculations will be used to determine the causes of this underprediction of wet scavenging. Additional comparisons will use other observations (Miller *et al.*, 2000; Harman-Fetcho *et al.*, 2000) and this evaluation will be completed during FY-2001.

Research and development will continue in FY-2001 toward the production of a CMAQ/atrazine version for public release. Work will also be performed to expand the model to handle other semi-volatile compounds such as polychlorinated dibenzo-para-dioxins and other dioxin-like compounds.

### **2.2.3.2 Atmospheric Mercury Field Research**

The Florida Atmospheric Mercury Study (FAMS) was conducted to characterize the atmospheric loadings of mercury to Florida (Guentzel, 1997). This study developed a simple box model that suggested the dominant source of mercury in rainfall to south Florida was from trade wind (long-range) transport from the Atlantic Ocean. The South Florida Atmospheric Mercury Monitoring Study (SoFAMMS) was conducted to investigate potential source-receptor relationships between anthropogenic point-source emissions in southeast Florida and atmospheric wet deposition of mercury (Dvonch *et al.*, 1998). This study used a multivariate source apportionment approach and concluded that approximately 70 percent of the mercury in

rainfall to southeast Florida was from waste incineration and oil combustion sources. The FAMS and SoFAMMS studies both identified atmospheric wet deposition as the dominant pathway for mercury into the Florida Everglades. The magnitude of local anthropogenic source contributions, however, remains a subject of contentious debate. Both studies highlighted the importance of reactive gaseous mercury (RGM) and meteorological transport in explaining the transport and deposition of mercury to south Florida. However, methods for measuring ambient concentrations of RGM were not available for the FAMS and SoFAMMS studies.

Reliable methods for discriminative measurement of ambient RGM and  $\text{Hg}^0$  have since been developed using annular denuder technology. Automated RGM monitoring systems are now available (*e.g.*, <http://www.tekran.com/access/1130.html>). In FY-2000, this new annular denuder technology was used on a research aircraft in a manual sample collection mode to evaluate the FAMS study hypothesis of long-range transport of RGM to Florida in the marine free troposphere. In a cooperative effort involving personnel from the Division, NOAA, ARL Silver Spring, Maryland, and the EPA National Exposure Research Laboratory, Research Triangle Park, North Carolina, a NOAA DeHavilland Twin Otter (DHC-6-300) aircraft was used to obtain measurements of RGM,  $\text{Hg}^0$ , and other ancillary measurements, in upwind air off the coast of Florida during mid-January to mid-February and during June of 2000. Ancillary measurements of ozone ( $\text{O}_3$ ), carbon monoxide (CO), sulfur dioxide ( $\text{SO}_2$ ), nitrogen oxides ( $\text{NO}$ ,  $\text{NO}_x$ ,  $\text{NO}_y$ ), condensation nuclei (CN), and various trace elements in aerosol form were also collected to be used to identify sources of observed RGM. The data collected were subject to QA/QC procedures at ARL Headquarters during FY-2000. A cooperative effort to analyze these data and arrive at scientific conclusions about the source of RGM impacting south Florida will continue through FY-2001.

#### **2.2.4 Meteorological Modeling Studies**

The fifth-generation Penn State/NCAR Mesoscale Model (MM5) is the primary tool for providing meteorological input for Models-3/CMAQ. MM5 is widely used for providing meteorological characterizations throughout the air quality modeling community. For Models-3/CMAQ, MM5 is applied to several case studies at a variety of spatial scales using a series of one-way nested domains. MM5 is run retrospectively using four-dimensional data assimilation (FDDA) for a dynamic analysis of the simulation period. The output represents a dynamically consistent multiscale meteorology simulation for continental scale (*e.g.*, either 108 km or 36 km), regional scale (*e.g.*, 36 km, if 108-km simulation is made), mesoscale (*e.g.*, 12 km), and urban scale (*e.g.*, 4 km). A 108-km simulation is performed if the background analyses used as input to the MM5 pre-processing have a coarse (*e.g.*,  $2.5^\circ$  latitude/longitude) horizontal grid spacing as is typical of archived global meteorological model output. The three finest resolutions are then run through the CMAQ emissions and chemistry modules.



#### 2.2.4.1 Meteorology Modeling for Models-3/CMAQ Applications

Several projects were underway during FY-2000 using MM5 to support Models-3/CMAQ applications. MM5 Version 3 (MM5v3) was released by the National Center for Atmospheric Research (NCAR), Boulder, Colorado, in late FY-1999, and it was tested for air quality applications. MM5v3 includes major changes to the NCAR code in MM5v2, including a new input/output format, a year-2000-compliant date structure, and formal support for the software on various serial and parallel hardware architectures. MM5v3.3, released by NCAR in January 2000, was predominantly used in FY-2000, and MM5v3.4, to be released by NCAR in November 2000, will be used in FY-2001. MM5v3.3 was tailored for air quality applications with some minor modifications. The significant changes made to the NCAR release include standardizing the radius of the earth with the emissions and chemistry modules, enabling analysis nudging FDDA and initialization from one-way nesting to occur in the same simulation, and changing to the planetary boundary layer parameterization. With the exception of projects started prior to the release of MM5v3 from NCAR, the Division has fully transitioned to MM5v3, and the majority of utility code updated to accommodate the new MM5v3 output format.

During FY-2000, initial testing of MM5v3.3 involved using Eta Data Assimilation System (EDAS) analyses from the National Centers for Environmental Prediction (NCEP). The EDAS analyses are archived for a domain over most of North America with full three-dimensional fields at 3-hourly intervals on a horizontal grid spacing of 40 km. This represents a significant improvement in temporal and spatial resolution over the 2.5° latitude/longitude at 12-hourly interval analyses that were previously used. Since the horizontal grid spacing is dramatically improved using EDAS, the 108-km MM5 domain was eliminated, and the 36-km domain was set to cover the continental United States. The test case for MM5v3.3 was July 13–30, 1998, selected to coincide with air quality simulation for an isoprene photochemical field study. MM5v3.3 was executed in four 4.5-day runs (including a 12-hour spin-up period in each run). A significant effort was placed on quality control of the new processors in MM5v3.3 and the EDAS analyses. MM5 successfully captured the placement of the oscillating stationary front and precipitation patterns through the period. The integration and trouble-shooting exercise using MM5v3.3 and EDAS was presented (Otte, 2000) at the Tenth PSU/NCAR Mesoscale Model Users' Workshop. The MM5 simulations were also used for two studies (Schwede *et al.*, in press; Pleim *et al.*, in press) that were presented at The Sixth International Conference on Air-Surface Exchange of Gases and Particles, Edinburgh, United Kingdom. The CMAQ simulations for the isoprene study have not been performed.

Another research effort in FY-2000 was to use FDDA based on observation nudging in high-resolution MM5 runs. Using the July 1995 NARSTO-NE cases established in FY-2000, the observation nudging was implemented for sensitivities on a large 4-km domain covering the northeastern United States. More than 100 surface observation sites were available, as were radiosonde soundings and wind profilers. By partitioning the data into two sets (one for nudging and the other for verification), a series of simulations was performed to set user-definable parameters for observation nudging. Those parameters were applied to the full set of observations to generate an improved set of runs at 4-km for July 1995. Work with new

observation nudging strategies will continue in FY-2001 as higher-resolution runs are considered.

Lastly, a preliminary demonstration of anisotropic weighting functions in FDDA was completed in FY-2000. The research used an observing-system simulation experiment to illustrate that anisotropic weighting functions have subtle but important impacts in FDDA. The results of this research appear in Otte *et al.* (accepted for publication). An extension of this work to air quality modeling is planned.

#### **2.2.4.2 Advanced Land-Surface and Planetary Boundary Layer Modeling in MM5**

MM5 was coupled to an advanced land-surface and PBL model to improve simulation of surface fluxes and PBL characterization. Such surface and PBL quantities as surface air temperature and PBL height are critical to realistic air quality modeling. The new land-surface model, known as the PX LSM (Pleim and Xiu, 1995; Xiu and Pleim, accepted for publication), includes explicit soil moisture and vegetative evapotranspiration along with ACM (Pleim and Chang, 1992). The FY-2001 effort was dominated by collaboration with the MMM group at NCAR toward the MM5v3.4 release in November 2000, which includes the PX LSM as one of two LSM options. Evaluation and improvement through comparison to field experiment data also continued in FY-2000.

The PX LSM is fully integrated in the NCAR-supported MM5v3.4 as a beta release. No modifications are necessary to MM5 preprocessor programs. However, certain options in Terrain are necessary to produce gridded fractional information of land use and soil type. Also, a new preprocessor *InitPX* is provided to process initial fields of soil moisture and soil temperature from previous model runs so that a continuous simulation over many multi-day runs can be made. Instructions for use of the PX LSM can be found in the MM5 tutorial that is on the NCAR MM5 website at <http://www.mmm.ucar.edu/mm5/mm5-home.html>.

Evaluation and further improvement of the PX LSM through comparison to field experiment data is continuing. In addition to previous studies comparing model runs to surface fluxes over corn, grass, and soybeans, case studies were made for a mixed deciduous-coniferous forest field study in the Adirondack area of New York in July 1998, and two sites, grass and soybeans, near Nashville, Tennessee, that were part of the SOS 1999 field study. These comparison studies included evaluation of such meteorological parameters as surface level temperature, and humidity, and surface fluxes of heat, moisture, and net radiation as well as ozone dry deposition velocity from a dry deposition model that couples to the PX LSM. The results of these studies were presented at a meeting in Edinburgh, Scotland, in June 2000, and will be published in a special issue of *Water, Air, and Soil Pollution* (Pleim *et al.*, in press). Such comparisons to field surface flux and meteorology measurements are extremely valuable for improvement of the model's applicability to simulate a variety of vegetation types.

A new feature in the latest modeling study for the SOS 1999 field study is an upgraded version of the ACM PBL model called ACM2. Rather than direct non-local transport from layer one to all other layers in the convective boundary layer, as in ACM, ACM2 includes a physical surface layer defined by the Obukhov Length. Within the surface layer, mixing is accomplished by eddy diffusion using eddy diffusion coefficients defined by surface layer similarity theory. Above the surface layer, non-local mixing is applied in the same manner as in the ACM. ACM2 can better represent the surface based super-adiabatic layer since it can be multi-layer with a physical definition. ACM2 will also be applied to CMAQ, where it will result in more gradual mixing of surface emissions than in the ACM.

## **2.2.5 Dry Deposition Studies**

### **2.2.5.1 Dry Deposition Research**

#### **Field Studies.**

An analysis of dry deposition data from three forest field studies was completed. The forests were in central North Carolina, northwestern Pennsylvania, and the Adirondack region of New York. The study included a thorough description of deposition processes to forests, and an evaluation of the performance of the multi-layer deposition velocity model in a forest environment. A journal article on the studies was published (Finkelstein *et al.*, 2000).

The study found that average daily deposition velocities are quite similar among sites. For  $O_3$ , they are 0.75, 0.75, and 0.79 cm/s at Kane Forest, Pennsylvania; Sand Flats, New York; and Duke Forest, North Carolina, respectively. For  $SO_2$ , they are 1.04 and 1.01 cm/s at Kane and Sand Flats. The seasonal cycles of  $O_3$  deposition velocity are pronounced, and closely follow the green up and senescence of the foliage. The seasonal cycle for  $SO_2$  deposition velocity shows less variation between spring, summer, and fall, but still shows the effects of vegetative uptake superimposed on year-round surface uptake. Because the concentrations of  $SO_2$  in remote areas are usually substantially less than those for  $O_3$ , the fluxes of  $O_3$  are usually higher.

Average daytime values for  $O_3$  deposition velocity over forests peak in mid-morning when stomatal activity is greatest, and not near noon as it does over crops or as  $SO_2$  deposition velocity does over crops and forests. Minimum values of deposition velocity for both  $SO_2$  and  $O_3$  occur early in the night, and then tend to slowly increase, perhaps due to surface absorption caused by increases in wetness and/or early opening of the stomata. Even before any light reaches the trees, stomata may be open in some species, resulting in some uptake throughout the night. This was observed at the mixed and pine forests sites, but not at the deciduous forest sites.

A comparison of the average daily maximum deposition velocity during fast growth periods with similar results over crops indicates that maximum  $O_3$  deposition velocity is higher to forests than to corn or pasture, but about the same to the more dense soybeans.  $SO_2$  deposition velocity to forests is only slightly higher than it was to corn or pasture, but less than to soybeans.

The ratio of SO<sub>2</sub> deposition velocity to O<sub>3</sub> deposition velocity is greater over crops than over forests.

### **Models.**

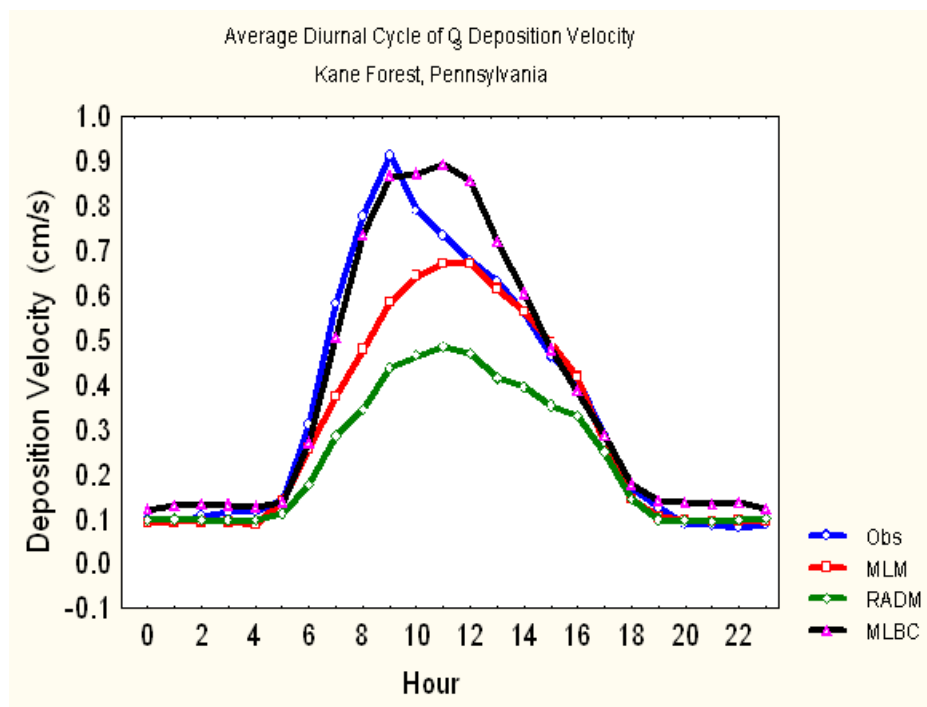
To help understand these processes, significant progress was made in developing the next generation deposition velocity model, which is called the Multi-Layer Bio-Chemical dry deposition model (MLBC). The model uses an improved Gaussian quadrature integration scheme, which reduces the number of layers needed in the integration and is more accurate; a significantly revised aerodynamic resistance model based on similarity theory; a simplified boundary layer resistance model; and a revised and enhanced short- and long-wave canopy radiation model. Stomatal resistance, rather than based on the typical Jarvis scheme, is based on a model of Farquhar *et al.* (1980), which calculates stomatal conductance by considering photosynthesis and respiration processes. This method provides more insights into the biochemical mechanisms governing photosynthesis and respiration, and how these are tied to stomatal conductance considering the direct and indirect effects of environmental factors.

MLBC also has a new cuticular resistance model. Plant cuticles are a lipophilic polymer membrane that consists of an insoluble bipolymer cutin and waxlike lipids. Diffusion across this layer can be either directly from the air to the layer, or from the air to a thin water film that usually exists on outdoor surfaces, and from the water layer to the cuticle. Diffusion equations for each of these pathways are developed that depend on the chemistry of the cuticle, water, and each pollutant.

Tests of this model against data collected in the field studies show significant improvement over the present generation of models. Figure 1 shows the average diurnal cycle of ozone deposition velocity observed over Kane Forest, and model results from MLM used in CASTNet, the RADM deposition model used in the present generation of Models-3/CMAQ, and the new MLBC. After its completion, MLBC will be modified for use in Models-3/CMAQ, and combined with other improvements in deposition velocity modeling discussed below.

### **Methods Evaluation.**

Atmospheric fluxes are controlled to a significant degree by atmospheric turbulence, and particularly by large eddies in the planetary boundary layer. These large eddies are somewhat random, stochastic events. Thus, observations of atmospheric fluxes over normal time periods, *i.e.*, 15 to 60 minutes, have a random error component that can be evaluated if the variance of the flux or covariance is known. The direct calculation of the variance of the covariance is a powerful and inclusive method for calculating the random sampling error in eddy correlation measurements. It takes into account sources of error not considered by previously published approaches, and as a consequence, tends to produce larger estimates for the error. For the approximately 100 samples taken from a variety of field programs over both low agricultural



**Figure 1.** Average diurnal cycle of O<sub>3</sub> deposition velocity observed over Kane Forest, Pennsylvania.

crops and forests, the normalized sampling error ranged from approximately 10% for sensible heat to 25%-30% for trace gases. These rather large sampling errors in flux measurements should be kept in mind when considering problems related to closing the energy balance, CO<sub>2</sub> budgets, or comparing deposition model results to measurements.

#### 2.2.5.2 Dry Deposition Modeling

As part of the CMAQ development, a new method for modeling dry deposition of gaseous chemical species was developed to take advantage of the more sophisticated surface model, PX LSM, implemented in MM5. Since PX LSM has an explicit parameterization for evapotranspiration, the same stomatal and canopy conductances can be used to compute dry deposition velocities of gaseous species. This technique has the advantage of using more realistic conductance estimates resulting from the integrated surface energy calculation where the soil moisture is continually adjusted to minimize model errors of temperature and humidity. The dry deposition model was previously evaluated for ozone deposition by comparing model results with field measurements at Bondville, Illinois, and Keysburg, Kentucky (Pleim *et al.*, 1996; Pleim *et al.*, 1997). Further evaluation studies were performed in FY-2000 for a 1998 mixed forest study in New York, and two sites, grass and soybeans, near Nashville, Tennessee, that were part of the SOS 1999 field study. Results of the forest study and a 1995 study for soybeans in Kentucky were presented at a meeting in Edinburgh, Scotland, in June 2000, and will be

published in a special issue of *Water, Air, and Soil Pollution* (Pleim *et al.*, in press). The impact of the new dry deposition model and PX LSM on the simulation of air chemistry by the CMAQ system was tested as part of the 1995 NARSTO-NE evaluation study. Results of this study were presented at the NATO/CCMS Millennium conference in May 2000 (Pleim and Byun, 2000).

## **2.2.6 Technical Support**

### **2.2.6.1 North American Research Strategy for Tropospheric Ozone**

NARSTO (formerly known as the North American Research Strategy for Tropospheric Ozone) is a coordinated 10-year research strategy to pursue the science-based issues that will lead to better management of the North American tropospheric ozone, particulate matter, and other air quality problems. It includes a management function for performing this coordination across the public and private sector organizations sponsoring air quality research, as well as those groups performing the research, including the university community. Canada and Mexico are also participating in the continental NARSTO program. During FY-2000, the ongoing NARSTO science assessment of tropospheric ozone was brought partially to completion, with the publication of a special NARSTO issue of *Atmospheric Environment* (2000). This Special Issue contains a set of Critical Review papers, commissioned specially for the ozone assessment that covers relevant areas including ambient measurements and networks, field studies, source emissions, atmospheric chemistry, and meteorological and air quality models. The second part of the ozone assessment, an Assessment Report (NARSTO Synthesis Team, in press) relating the state-of-science to outstanding air quality management issues, will be published in FY-2001.

### **2.2.6.2 Western Regional Air Partnership Air Quality Technical Forums**

The Western Regional Air Partnership (WRAP) is a broad-based regional air quality coordinating organization composed of States and Tribes in the western United States, U.S. Departments of Agriculture and Interior, EPA, and other affected stakeholders representing industry, environmental groups, and other interested parties. One Division scientist participated in the Air Quality Modeling Forum (AQMF) and Research and Development Forum (R&DF), which are two of several committees of WRAP formed to provide technical guidance. WRAP is a follow-on organization to the Grand Canyon Visibility Transport Commission, whose objective was to provide technical and policy input needed to regulate regional haze in the western United States. AQMF provides WRAP with technical analyses needed to meet practical, real-world objectives, especially as they relate to meeting the regulatory requirements of the EPA regional haze rule (RHR) published July 1, 1999. Specific AQMF modeling assessments on regional visibility include (1) relative incremental contribution of a given source or source control on visibility at one or more Class I areas; (2) cumulative impact of regional source growth or control on Class I areas throughout the region; (3) impact of regional sources during periods of high and low visibility conditions; and (4) evaluation of cost-effective alternatives for improving regional haze. Time frames required by the RHR are (1) near-term (SO<sub>2</sub> regional emission trading

program plan due October 1, 2000); (2) intermediate to long-term (additional requirements for regional visibility modeling by December 31, 2003); and (3) long-term (modeling to support SIPs due no later than December 31, 2008). WRAP AQMF is using Models-3/CMAQ for performing the intermediate- and long-term modeling for RHR. R&DF is sponsoring the development of science modules to handle fugitive dust emissions in CMAQ. A workshop based on technical recommendations from an expert panel is planned for December 2000.

#### **2.2.6.3 Multimedia Integrated Modeling System Meteorological Team**

Accurate characterization of the atmosphere is an essential part of any environmental modeling endeavor. During the development of the Multimedia Integrated Modeling System (MIMS), research will be ongoing to improve this characterization and its seamless integration into MIMS. MM5v3 is used to generate meteorological data for CMAQ; however, additional models will also be considered in the future. Two problems common to the meteorological models are the intensive computations involved because of their complexity and the tremendous amounts of data generated. These constraints are exacerbated with MIMS, because unlike episodic air quality studies, which typically simulate 10-day periods, MIMS will be required to perform much longer simulations to study the impact of nitrogen loading to the watershed. As a result, such statistical approaches as aggregation may be required. Such a procedure was applied successfully to air quality studies in the past, including CMAQ simulations (Cohn *et al.*, 1999; Eder *et al.*, accepted for publication; Cohn *et al.*, in press). With aggregation, a limited set of meteorologically representative time periods are used to derive the required seasonal and annual estimates. Therefore, in practice, MM5 and MIMS may have to be executed for finite episodes or events, the results of which would be aggregated to achieve the requisite seasonal or annual results.

#### **2.2.6.4 Climatological and Regional Analyses of CASTNet Data**

The spatial and temporal variability of ambient air concentrations of  $\text{SO}_2$ ,  $\text{SO}_4^{2-}$ ,  $\text{NO}_3^-$ ,  $\text{HNO}_3$ ,  $\text{NH}_4^+$  and  $\text{O}_3$  obtained from the EPA Clean Air Status and Trends Network (CASTNet) was examined using an objective, statistically based technique called rotated principal component analysis. This analysis, which covered the period October 24, 1989, through August 15, 1995, allowed for the identification and subsequent characterization of homogeneous influence regimes associated with each of the six species. This identification of homogeneity across sites has added to the weight of evidence supporting regionality of species behavior, which has historically been difficult to estimate and understand because of complicating meteorological and chemical factors.

Depending on the species, either two ( $\text{NO}_3^-$ ); three ( $\text{SO}_2$ ,  $\text{SO}_4^{2-}$ ,  $\text{NH}_4^+$ ,  $\text{O}_3$ ); or four ( $\text{HNO}_3$ ) influence regimes were identified by the analysis. Examination of the temporal variability of these homogeneous influence regimes through time series and spectral analysis revealed various seasonal and annual cycles of differing strengths and timing. Examination of these differences

facilitated understanding of both the meteorological and chemical atmospheric processes that are responsible for the regimes (Eder and Sickles, in press).

This analysis provided evidence of, and considerable insight into, the regional-scale behavior of these species' air concentrations, which suggests that exclusively local strategies to reduce their concentrations through reductions in emissions may be wholly inadequate without parallel management of regional emissions. Such region-wide, homogeneous patterns seen over the eastern United States will require interstate strategies for the reduction of these pollutants.

#### **2.2.6.5 NEXRAD Stage IV Data in the Multimedia Modeling of Pollutant Transport**

MIMS is being designed to model the cycling of pollutants and nutrients between the atmosphere and the earth's surface, including water bodies and groundwater. The ability to accurately model both atmospheric, hydrological, and surface processes that transport chemicals is highly dependent on precipitation types, rates, and totals. Of special interest are precipitation extremes and subsequent flooding, which can greatly enhance the movement of such chemicals. During such events, these chemicals can enter the surface water bodies via groundwater recharge as well as overland flow. For example, the extreme 1999 flooding of North Carolina associated with Hurricane Floyd, transported tremendous amounts of agricultural and industrial waste and pesticides into area estuaries and rivers. This Hurricane, which followed Hurricane Dennis, inundated sections of eastern North Carolina with more than 20 inches of rain.

During the development of MIMS, the use of the National Weather Service NEXRAD (NEXt generation RADar) Stage IV precipitation estimates in modeling efforts is being investigated. The NEXRAD Stage IV data consist of precipitation data fields that have assimilated both rain gauge data and WSR-88D (Weather Surveillance Radar 1988 Doppler Version) data into a comprehensive hourly, national data set with a 4-km<sup>2</sup> resolution. The purpose of this research is to evaluate the quality and identify limitations of the NEXRAD data through a comparison with ground truth data obtained from a network of 10 closely spaced rain gauges. The evaluation will use visualization tools and statistical analyses to determine if the spatial resolution of NEXRAD data is adequate to capture the spatial variability of precipitation on the watershed that is used in the surface hydrology models associated with MIMS (Eder *et al.*, accepted for publication).

### **2.3 Modeling Systems Analysis Branch**

The Modeling Systems Analysis Branch supports the Division by providing routine and high performance computing support needed in the development, evaluation, and application of environmental models. The Branch is the focal point for modeling software design and systems analysis in compliance with stated Agency requirements of quality control and assurance, and for conducting research in the interagency Information Technology Research and Development (ITR&D) program (formerly High Performance Computing and Communications), which



includes parallel processing, visualization, advanced networking, and information management. Under the ITR&D program, the Branch is developing a flexible multi-media environmental modeling and decision support tool to deal with multiple scales and multiple pollutants simultaneously; thus, facilitating a more comprehensive and cost-effective approach to related single- and multi-stressor human and ecosystem problems.

### 2.3.1 Emission Modeling

The principal development in emission processing capability during FY-2000 was the Personal Computer (PC) with Microsoft® Windows™ NT<sup>3</sup> release of Models-3 Version 4 during the summer of 2000. The Models-3 Emission Processing and Projection System (MEPPS) was enhanced and stabilized by testing and debugging. In addition, work continued on MEPPS replacement, the Sparse Matrix Operator Kernel Emission (SMOKE<sup>4</sup>) system. Specific developments included:

- The Models-3 Version 4 release (June 30, 2000, for the NT port) updated the Sun<sup>TM5</sup> UNIX<sup>6</sup> port of the system using the Solaris 2.7 operating system<sup>TM7</sup>, and updated the aerosol portions (aerosols 2) of the chemical mechanism options.
- The SMOKE processing system was extensively streamlined and modified for use in the Models-3 framework. SMOKE was initially developed as a prototype by the MCNC-North Carolina Supercomputing Center in cooperation with the Division (Houyoux and Vukovich, 1999). Its sparse matrix approach to the repetitive computations using very large emission databases decreases processing time by at least an order of magnitude. SMOKE was modified for incorporation and compliance within the Models-3 framework, unlike MEPPS, which is a SAS<sup>TM8</sup>-based system that can only be semi-compliant and requires much more data file space. Substantial data handling and quality control capability will be added to SMOKE to make it fully functional in Models-3. In addition,

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<sup>3</sup>Microsoft and Windows NT are registered trademarks of Microsoft Corporation; and NT is a registered trademark of Northern Telcom Limited.

<sup>4</sup>Copyright 1999 MCNC-North Carolina Supercomputing Center, Research Triangle Park, NC.

<sup>5</sup>Sun is a trademark of Silicon Graphics, Inc.

<sup>6</sup>UNIX is a trademark of AT and T.

<sup>7</sup>Solaris 2.7 operating system is a trademark of Sun Microsystems.

<sup>8</sup>SAS is a registered trademark of SAS Institute, Inc.

an input file quality control and file formatting tool (SMOKE Tool) is being developed because SMOKE cannot create its own input files and grids from diverse sets of raw data.

- A software interface was developed to allow the use of the Pesticide Emission Model<sup>9</sup> (PEM) with SMOKE, under an agreement between the Agency and Ortech International, Mississauga, Ontario, Canada, the developers of PEM. To be operational in Models-3, the Models-3 Meteorological Chemistry Interface Processor (MCIP) needs to be modified and soil and vegetation databases added. PEM will allow a user to model hourly episodic pesticide emissions on a regional basis, consistent with geographic grids, meteorology data, and soil and vegetation data.
- MEPPS generated multiple emission data sets from July 2–18, 1995, for evaluation runs of CMAQ for spatial domains covering the eastern half of the United States and Canada. These emission data sets were produced at 36 km, 12 km, and 4 km, with some tests at 1.3-km spatial resolution for both CB-IV and RADM2 lumped species model chemistry approaches.

### 2.3.2 Biogenic Emissions

The Branch continues to develop and test algorithms for simulating airborne emissions from natural and biogenic sources. These sources include hydrocarbons from vegetation, nitric oxide and ammonia from soils, nitric oxide from lightning, and ammonia from livestock operations. The algorithms will be integrated into the Biogenic Emissions Inventory System (BEIS), the third generation of which should be released during FY-2001.

The basis for BEIS3 was reported in a NARSTO critical review article (Guenther *et al.*, 2000). BEIS3 will produce hourly, gridded emission fluxes for 34 chemical species, including 14 monoterpenes. It is thought that this enhanced speciation will help in modeling the secondary formation of organic aerosols. Late in FY-2000, Division scientists began to incorporate BEIS3 into the SMOKE emission modeling system. Testing of SMOKE/BEIS3 in CMAQ will begin during early 2001.

A presentation at the Global Climate and Hydrology Center in Huntsville, Alabama, highlighted the possible importance of lightning-produced nitric oxide for regional air quality modeling (<http://www.epa.gov/asmdnerl/biogen.html>). A simulation with RADM indicates that lightning may contribute ~10 percent of total nitrogen oxide (NO<sub>x</sub>) emissions during the summer in the eastern United States. This finding could be important because lightning NO<sub>x</sub> is not explicitly included in most regional model simulations.

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<sup>9</sup>Copyright to CGEIC ORTECH and licensed to users by Ortech International.

A web site was created to provide additional information on the Division's biogenic emissions research, slides of presentations, and access to data and computer algorithms. The web address is <http://www.epa.gov/asmdnerl/biogen.html>.

### **2.3.3 Improvements in Vegetation Cover Data**

Regional air quality models need accurate characterization of vegetation cover to estimate biogenic emissions and dry deposition. However, most satellite-derived data sets, while providing good spatial resolution, do not resolve vegetation species and crop types. Isoprene emissions vary among tree species, with extremely high emissions from oaks, but negligible emissions from maples. Division scientists have constructed a 1-km vegetation database for North America, called the Biogenic Emissions Land use Database (BELD3). The USGS 1-km land-use/land-cover (LULC) data set derived from the NOAA Advanced Very High Resolution Radiometer (AVHRR) satellite imagery was coupled with forest inventory data from the U.S. Forest Service and the 1992 Agricultural Census. The 1990 Census was used to denote urbanized regions. Each 1-km pixel includes percent forest cover, percent crop cover, Federal Information Processing Standard code, and the USGS LULC class. In the United States, each pixel is further divided into tree species and crop types. This data set provides much greater spatial resolution than earlier county-based land-use data sets developed for biogenic emission calculations. It should provide a more accurate basis for vegetation-sensitive calculations for such regional air quality models as CMAQ. The data set can be accessed at <http://www.epa.gov/asmdnerl/biogen.html>.

### **2.3.4 Technology Transfer**

The release of Models-3/ CMAQ version 4 for the PC with a Windows<sup>TM</sup> NT<sup>®</sup> operating system occurred July 28, 2000. Installation is simpler on the NT<sup>®</sup> than on a UNIX<sup>®</sup> platform. An installation screen is used and installation uses CD-ROMs rather than tape. The version for the Windows<sup>TM</sup> NT<sup>®</sup> port is distributed by the National Technical Information Service (<http://www.ntis.gov/fcpc/cpn8867.htm>) and may be ordered online. In addition, a stand-alone version (science algorithms, supporting processors, and tutorial input files, but without the Models-3 framework), was made available by anonymous ftp (<ftp://ftp.epa.gov/amd>). Although many sites have downloaded the stand-alone version, there is no exact count. It is known that the stand-alone version, which was provided to run on a Sun workstation, was adapted by the user community to execute on other UNIX<sup>®</sup> platforms, including SGI<sup>TM10</sup> and DEC<sup>TM</sup> Alpha<sup>TM11</sup>. Models-3 documentation can be obtained at <http://www.epa.gov/asmdnerl/models3>.

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<sup>10</sup>SGI is a trademark of Silicon Graphics, Inc.

<sup>11</sup>DEC and DEC Alpha are registered trademarks of Digital Equipment Corporation.

#### 2.3.4.1 Visualization and Analysis Tools

Models-3/CMAQ is distributed with visualization tools that are integrated into the framework, including recent versions of PAVE<sup>©12</sup> (Package for Analysis and Visualization), available at [http://envpro.ncsc.org/EDSS/pave\\_doc/Pave.html](http://envpro.ncsc.org/EDSS/pave_doc/Pave.html); and Vis5D<sup>©13</sup>, available at <http://www.ssec.wisc.edu/~billh/vis5d.html>. The IBM<sup>®</sup> DX7<sup>®14</sup>, was not distributed with version 4. To use the visualization software in a Microsoft<sup>®</sup> Windows<sup>™</sup> NT<sup>®</sup> computing environment, the UNIX computing environment must be emulated using Microsoft<sup>®</sup> Interix<sup>™15</sup> (<http://www.interix.com/products/matrix.html>).

#### 2.3.4.2 Models-3 Workshop

A workshop was held in Arlington, Virginia, June 12-14, 2000. Over 200 attendees heard presentations of user experiences using Models-3/CMAQ along with evaluation results and plans for future direction. Part of the conference focused on the plan to establish and fund an institution that would provide Models-3/CMAQ support, develop and integrate new science, and assist in the transfer of the Models-3 technology to the air quality modeling community. The institution would be funded through a 4-year cooperative agreement with the intent of the institution becoming self-sufficient. Presentations from the workshop can be found at <http://www.epa.gov/asmdnerl/models3/workshop/agenda.html>.

#### 2.3.4.3 Models-3 Support

A Help Desk was established for Models-3/CMAQ. The Help Desk has a support structure consisting of a collection of individual scientists to answer user questions in specific areas. The telephone number for the Help Desk is 919-541-0157. The Models-3/CMAQ website (<http://www.epa.gov/asmdnerl/models3/>) was expanded to provide user support for a stand-alone version, *i.e.*, without the Models-3 framework. These codes may be downloaded and adapted to execute on any computing platform. The downloaded files contain code that ingests the data sets for a second tutorial designed to use the CB-IV chemical mechanism. The web site also contains

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<sup>12</sup>Copyright1997-2000 MCNC North Carolina Supercomputing Center, Research Triangle Park, NC.

<sup>13</sup>Copyright1990-1999 W. Hibbard, J. Kellum, B. Paul, D. Santek, and A. Battaiola.

<sup>14</sup>IBM is a registered trademark of the International Business Machines Corporation. IBM DX Visualization Data Explorer is a registered trademark of International Business Machines Corporation; Open-source availability starting May 26, 1999.

<sup>15</sup>Interix is a trademark of Softway systems, Inc.

*Model Change Bulletins* where known problems with the system are listed along with the instructions to solve the problem. Models-3 *Public Forum* area was established on the SCRAM (Support Center for Regulatory Air Models) web site (<http://www.epa.gov/scram001>). This area provides a central location for the discussion of issues related to the operation and use of Models-3. A listserv<sup>®16</sup> was established to which Models-3 users can subscribe and communicate with others by sending messages to [m3list@tempest.rtpnc.epa.gov](mailto:m3list@tempest.rtpnc.epa.gov).

#### **2.3.4.4 Computing Platforms for the Models-3 Framework**

The Models-3 framework was released only for Sun<sup>™</sup> workstations and Microsoft<sup>®</sup> Windows<sup>™</sup> NT<sup>®</sup> operating system. The framework has encountered problems with performance and licensing of Orbix<sup>™17</sup>, a commercial software component of the framework supporting distributed applications using object-oriented client-server technology. Future development of Models-3 framework will be directed away from the use of products that require licensing fees to the runtime user. The science code can be run on a number of machines and operating systems, including Sun<sup>™</sup>, DEC<sup>™</sup> Alpha<sup>™</sup>, Cray<sup>®</sup> C90<sup>™</sup>, Cray<sup>®</sup> T3E<sup>™18</sup>, SGI<sup>™</sup>, and Microsoft<sup>®</sup> Windows<sup>™</sup> NT<sup>®</sup>.

The scientific evaluation of CMAQ is being done on multiple computing platforms through the Models-3 framework. The modeling of emissions with MEPPS is being done on Sun workstations, and the MM5 simulations are being done on a Cray<sup>®</sup> C90<sup>™</sup>. CMAQ runs on a Cray<sup>®</sup> T3E<sup>™</sup> with the initial and boundary conditions being executed on either a Sun workstation or a Cray<sup>®</sup> C90<sup>™</sup>. Fortran 90 is used with the releases in FY-2000. The Fortran source code for the science modules is the same for multiple computing platforms, and is recompiled and linked on the host machine to create an executable for the specific host hardware. The use of a single scientific source code simplifies the management and maintenance of the software.

#### **2.3.5 Cross-Platform Implementation of CMAQ Chemistry-Transport Model**

Hundreds of CMAQ model runs are required, demanding rapid turnover for model evaluation, sensitivity studies, and other applications. The only computing platform that can meet the requirement is the Cray<sup>®</sup> T3E<sup>™</sup>, a distributed memory, high performance parallel computer. To take advantage of its performance capabilities, CCTM, ECIP, and ICON were modified to run in parallel. The modifications are sufficiently general, using a standard

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<sup>16</sup>Listserv is a registered trademark licensed to L-Soft International, Inc.

<sup>17</sup>Orbix is a registered trademark of IONA Technologies Ltd.

<sup>18</sup>Cray is a registered trademark and Cray C90 and Cray T3E are trademarks of Cray Research.

message-passing protocol that can run on any distributed memory architecture, including workstation farms or PC clusters.

The parallel implementation developed for CMAQ requires a horizontal grid domain decomposition involving near-neighbor communication (data transfer between adjacent processors) and file input/output (I/O) with data redistribution depending on processor location in the domain decomposition. The I/O is built on top of (layered on) the Models-3 I/O application programming interface. To manage and simplify the near-neighbor communication from the user's point of view, a stencil exchange library was developed that contains data communication calls, which can be inserted in the code.

The code modifications from the serial version necessary for the parallel version are not trivial, and the issue of code maintenance and control demanded a solution to the problem that arises from maintaining the same essential science algorithms, but implemented on different architectures. The solution developed for CCTM consists of:

- A single source code that contains a few precompiler options that are selected for execution on either serial or parallel platforms;
- The use of parallel I/O and stencil exchange libraries linked in at the load step during code compilation;
- Additions to existing Fortran including files containing the horizontal grid parameters associated with the domain decomposition; and,
- Additional pre-compiler directives to select the appropriate stencil exchange and parallel I/O functions during the compile phase.

To simplify the compilation and linking for different platforms, UNIX<sup>®</sup> 9 C Shell scripts were developed, and the monocode was successfully tested on the Cray<sup>®</sup> T3E<sup>™</sup> and Cray<sup>®</sup> T3D<sup>™</sup>, the Cray<sup>®</sup> C90<sup>™</sup>, Sun<sup>™</sup> and SGI<sup>™</sup> workstations, and PC Windows<sup>™</sup> NT<sup>®</sup>.

### **2.3.6 Multimedia Integrated Modeling**

The Branch is involved in a long-term project to develop a Multimedia Integrated Modeling System (MIMS). The MIMS software framework is being designed to comprehensively simulate the cross-media transport and fate of nutrients and chemical stressors over multiple and disparate scales. This system will provide a computer-based problem solving environment for studying such multimedia (atmosphere, land, water) environmental problems as over-loading of nutrients to aquatic ecosystems, which can result in anaerobic conditions and fish kills. As a test case, a multimedia model prototype is being designed to simulate the atmospheric, surface, and subsurface loading of nitrogen and the resulting effects on aquatic ecosystems and water quality of the Neuse River Estuary. The MIMS framework will provide

advanced tools to build, couple, and execute the individual process models; to coordinate the transfer of data between these models; and to visualize and analyze results.

The MIMS architecture design team was formed in FY-2000 and includes members from the Branch, EPA, and contractors. The team identified goals and desirable attributes for the MIMS framework, a software infrastructure for constructing, composing, executing, and evaluating cross-media models. The team also identified MIMS stakeholders and considered how MIMS might help them better accomplish their work. Based on that information, the team developed a draft MIMS software architecture, which it reviewed with interested groups. The architecture team explored technologies that could be used to implement the framework, including languages, object databases, and other modeling frameworks. The team decided that the framework will be implemented in Java, which is portable across platforms and often allows software to be developed with less effort than languages such as C and C++. The team is considering the use of the Dynamic Information Architecture System (DIAS), which was developed by Argonne National Laboratory, Argonne, Illinois. DIAS provides a paradigm and tools for coupling diverse models, including models that simulate physics, chemistry, and behaviors.

In parallel with the framework design is the design and initial development of a multimedia modeling prototype for the Neuse River Estuary. This is being coordinated by the Branch as follows:

- Upscaling of a spatially-explicit hydrology and nutrient cycling model (RHESSys or Regional Hydro-Ecological Simulation System). RHESSys was tested successfully at a variety of watersheds in past studies, and is being set up for several small instrumented watersheds within the Neuse River Basin. Because the spatially explicit approach may not be practical for the entire Basin, one or more approach(es) will then be suggested for upscaling RHESSys for the entire Neuse. The benefit from the spatially-explicit approach of RHESSys is that the regulatory modeling approaches cannot resolve the impact from localized (*i.e.*, sub-grid) land-use or vegetation changes (*i.e.*, riparian buffer zones) on nutrient loading. Sensitivity tests for such changes could help identify effective solutions when considering environmental management decisions.
- Coupling of a surface hydrology and meteorology model (MM5) to simulate the dynamic land-atmosphere flux of energy and moisture. This work is being extended to a small, instrumented watershed within the Neuse River Basin for testing.
- NWS NEXRAD (NEXt generation RADar) precipitation estimates will be provided in the MIMS system for a more accurate representation of precipitation than typically available from meteorological models on watershed scales.

- The Surface Water Object-Oriented Modeling System (SWOOMS) is being developed under an EPA grant for the Neuse River Estuary. SWOOMS will be able to simulate the hydrodynamics and water quality conditions that were correlated with fish kills in the Neuse River Estuary. The SWOOMS development began in FY-2000 and will be completed in FY-2003. The MIMS project is closely coordinated with this grant.
- Airborne ammonia emissions are a multimedia issue because the impact of such atmospheric conditions as temperature can affect the emission flux. However, emission inventories only provide annual estimates. For this reason, an inverse modeling study is underway to provide improved estimates of seasonal ammonia emissions, which should improve the air quality model's predictions of atmospheric deposition of nitrogen compounds for MIMS.

These efforts are being coordinated for incorporation into the MIMS multimedia model prototype. Annual workshops were held to bring EPA grantees together with MIMS researchers. In addition, a smaller working group was formed to meet on a quarterly basis for planning and review.

## **2.4 Applied Modeling Research Branch**

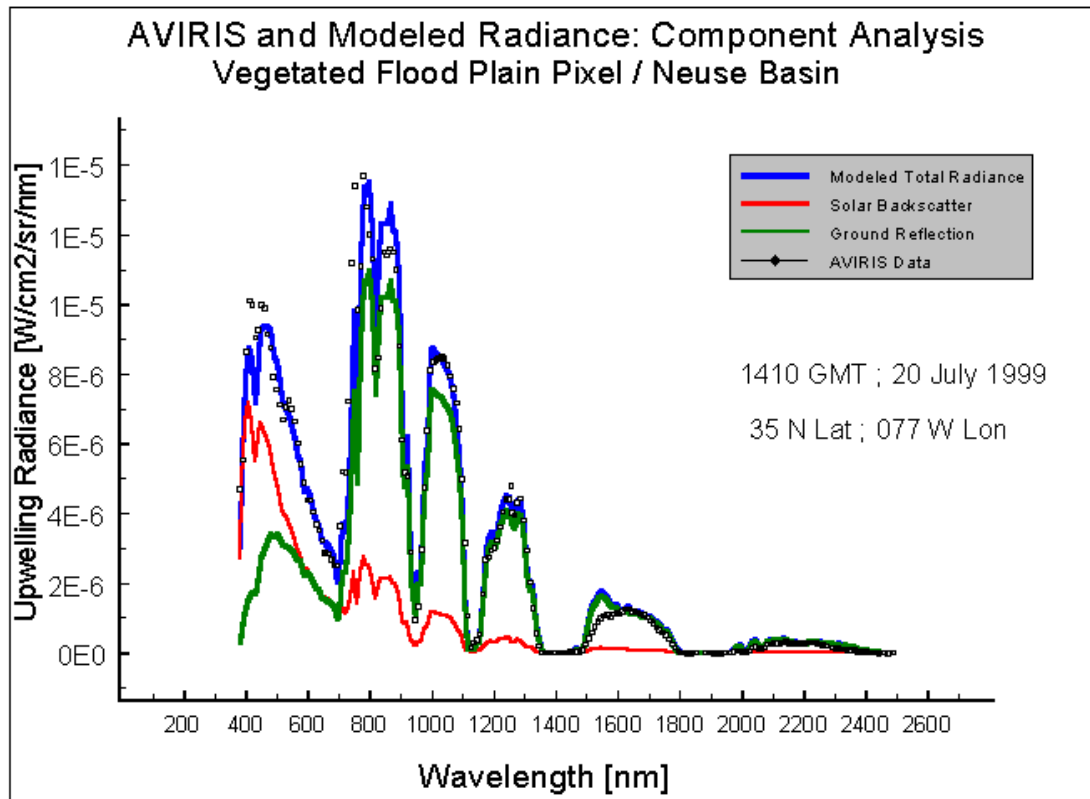
The Applied Modeling Research Branch investigates and develops applied numerical simulation models of sources, transport, fate, and mitigation of air toxic pollutants in the near field and conducts research to develop and improve human exposure predictive models, focusing principally on urban environments where exposures are high. Databases are assembled and used for model development and research on flow characterization, dispersion modeling, and human exposure. Using the Fluid Modeling Facility (FMF), the Branch conducts simulations of atmospheric flow and pollutant dispersion in complex terrain, in and around such obstacles as buildings, in convective boundary layers and dense gas plumes, and in other situations not easily handled by mathematical models.

### **2.4.1 Remote Sensing**

Large scale assessment of land use and ecological health is feasible only with remote sensing methods. One of the physical variables characterizing a landscape is its spectral albedo, or reflectance. The EPA Change Detection program is developing methodologies to extend remote sensing techniques to quantitative ecological assessments using NASA's Airborne Visible and Infrared Imaging Spectrometer (AVIRIS). The AVIRIS instrument is a nadir-looking spectral radiometer that measures upwelling radiance [ $\text{W/m}^2/\text{sr/nm}$ ] in 224 bands (nominal 10 nm bandwidth) from 370 nm to 2510 nm, with a spatial resolution of 20 m. It is typically mounted aboard a converted U2 Air Force aircraft and flown at altitudes of up to 20 km above sea level. Geo-coded images permit atmospheric correction by comparing an AVIRIS absolute radiance with co-located ground-truth reflectance spectra. The MODTRAN (MODERate



resolution TRANSMittance) radiative transfer model was employed for this task, calculating upwelling radiance for atmospheric conditions and geodesic configuration prevailing at the time of overflight. The lower Neuse River Basin is the first in a series of regions that will be characterized with respect to its land use and ecological state by the spatially-resolved reflectance (Figure 2).



**Figure 2.** Modeled and measured radiance spectrum of the flood plain in the Neuse River Basin, and component contributions from atmospheric backscatter and ground reflectance.

#### 2.4.2 Relating field-Scale Wind Blown Fugitive Dust Measurement to Large Scale Vertical Dust Flux

Work began on comparing measured concentrations of  $PM_{10}$  from fugitive dust sources to dust emissions from unpaved roads. A model of the diffusion and deposition of fugitive road dust was used. The model was presented at the Western Regional Air Pollution Expert Panel meeting in Ventura, California, on September 12-13, 2000 (<http://www.wrapair.org/commindex.htm>).

A lumped control volume approach was used to consider dust generated from a road surface. Two-dimensional symmetry, conservation of mass, and steady state conditions were assumed. A control volume was specified where none of the road dust passes through the control volume ceiling immediately above the road and is long enough for the flux of dust upwind of the road to be equal to the flux of dust through the downwind wall of the control volume. The equations for mass conservation, vertical diffusion through the ceiling of the control volume, and deposition at the floor of the control volume were solved. Equation 1 gives the dimensionless ratio  $\Phi$  of the vertical flux of fugitive dust transported in a regional scale model to the microscale vertical dust flux:

$$\Phi = \frac{K}{(V_d + K)} \quad (1)$$

The ratio given by Equation 1 can be approximated using data from Gillette (1974) showing  $K = 0.08u_*$ , where  $u_*$  is friction velocity. Values for  $V_d$  versus size and environmental conditions are given by Slinn (1982). The resulting dimensionless values for  $\Phi$  express the ratios of regional-effective fluxes of  $PM_{10}$  to the microscale vertical fluxes of  $PM_{10}$  at the source.

The expression given in Equation 1 partially explains why observed concentrations of  $PM_{10}$  produced by road dust are smaller than predicted by large grid-scale models. Large-scale models do not presently correct for local scale deposition, but rather use the entire amount of dust emitted by roads. Because dust is deposited to the surface close to the source, dust vertical fluxes not corrected by the ratio  $\Phi$  lead to overestimates of dust concentrations downwind of the source. Other expected effects are:

- Large-scale vertical flux of dust would be a very large fraction of field-scale flux of wind erosion dust from road surfaces.
- Dust devils should be considered effective sources of dust because dust devils have a high height of initial dust input, and  $\Phi$  for dust devils should be close to one. Gillette and Sinclair (1989) describe dust devil dust fluxes.

### 2.4.3 Fugitive Emissions from Supply-Limited Sources

Wind erosion mechanisms were investigated for the scrape site at the Jornada Experimental Range in the Chihuahuan desert near Las Cruces, New Mexico. The scrape site was denuded of vegetation and scraped flat in 1991. Three meteorological towers, each 2 m in height, with wind speed sensors at 0.2, 0.5, 1.0 and 2.0 m above ground; air temperature at 0.2 and 2 m height; rain gage; seven sets of particle collectors at 0.1, 0.5, and 1.0 m heights; and three fast-response particle mass flux sensors at 0.02, 0.1, 0.2, and 0.5 m heights were installed and operated for a period of 35 months along a transect crossing the site and parallel to the predominant southwesterly wind direction. The minimum threshold friction velocity for the

scrape site with a thin layer of loose material was  $25 \text{ cm s}^{-1}$ . This minimum threshold velocity increased to as high as  $100 \text{ cm s}^{-1}$ , depending on the degree of particle depletion and the site's status that varied between supply-unlimited just after a high-wind episode, and the more typical supply-limited. Sandblasting of the surface crust was the dominant mechanism producing fresh sediment for transport. The measurements showed that supply and availability of loose, fine particles on the surface is the predominant control of erosion rates rather than wind energy.

By measuring the horizontal sand flux, friction, and threshold friction velocities at three points on the Jornada scrape site, the sand flux could be related to the maximum potential flux, *i.e.*, the sand flux from a crust-free and vegetation-free surface with thick deposits of loose sand for the same winds. This approach using potential flux was derived from wind and sand flux measurements at Owens Lake (Gillette *et al.*, in press) for a thick layer of loose sand and no surface crust, *i.e.*, a supply unlimited surface. The potential sand flux was calculated by using the friction velocity of the wind and the threshold friction velocity. The difference between the actual sand drift and the potential sand drift is a measure of the effect of particle supply limitation.

Transport of sand from the scrape site was estimated based on the assumption that the direction of transport is to the northeast, which is the dominant wind direction for strong winds. It was further assumed that the source of new sand on the scrape site is abraded material from the crust. With these two assumptions, a simple model of transport of sand from the scrape site was developed. For large abrasion events, the amount of sediment cleared by wind transport is larger than for smaller events, but it is significantly smaller than particle production. Consequently, in months following a large abrasion event, there is still significant southwest-northeast sediment removal even if no new abrasion is taking place. This result would explain the observations that there were variable thicknesses of loose sand over time on the surface crust. Newly formed thick layers of sand would act like supply-unlimited sources. Eventually a thick layer of sand would be depleted by transport in the northeast direction. At some point during the removal stage the transport becomes more supply limited.

When the surface was covered by a thin layer of loose particles of one or more millimeters in size, the transport of sand from the surface by winds slightly over the threshold friction velocity would deplete the surface of loose material. However, winds strong enough to abrade the surface by sandblasting would supply the surface with fresh loose material. This abrasion mainly occurred in a few episodes above a threshold of about  $100 \text{ cm s}^{-1}$  that were capable of transporting particles larger than  $400 \mu\text{m}$ . The data showed that the observed transport rate is not as fast as the particle production for periods of large abrasion. However, for the 35 months of the experiment, transport was sufficient to remove most of the fresh material produced by sandblasting within about a month.

#### **2.4.4 Resuspension of PM<sub>10</sub> Particles from Grass**

Past research on the production of PM<sub>10</sub> by the wind has shown that the dominant, but not the only, mechanism is the transfer of kinetic energy to the surface by particles larger than 50 micrometers. The mechanism known as sandblasting by saltating grains utilizes sand-sized particles that are entrained by wind speed lower than those needed to entrain PM<sub>10</sub> particles directly. Since the sand-sized particles are only airborne for short periods of time, the collision with loose and bound PM<sub>10</sub> particles on the surface provides the primary energy transfer needed to produce the PM<sub>10</sub> particles. Research is underway to develop a detailed understanding of the mechanisms of resuspension from vegetation surfaces and to develop a mechanistic model to describe these processes. In previous years, a methodology was developed to quantify the conversion of wind energy to the mechanical energy of impaction and rubbing of a single grass blade. An instrument was found that gives linear response to kinetic energies from both rubbing motions and impaction of  $10^{-9}$  joules to  $10^{-7}$  joules. Wind tunnel experiments were conducted to test the quantity of PM<sub>10</sub> produced by impaction and rubbing of a grass blade. Turbulence characteristics in the wind tunnel were established using turbulence grids. A wheat grass was used along with a Grimm aerosol size distribution analyzer to test downwind aerosol concentrations of known-size polystyrene latex particles that were deposited on the surface of a grass blade. Following the analysis of this experimental work, models will be built for the resuspension of PM<sub>10</sub> from surfaces that are bare or covered by vegetation.

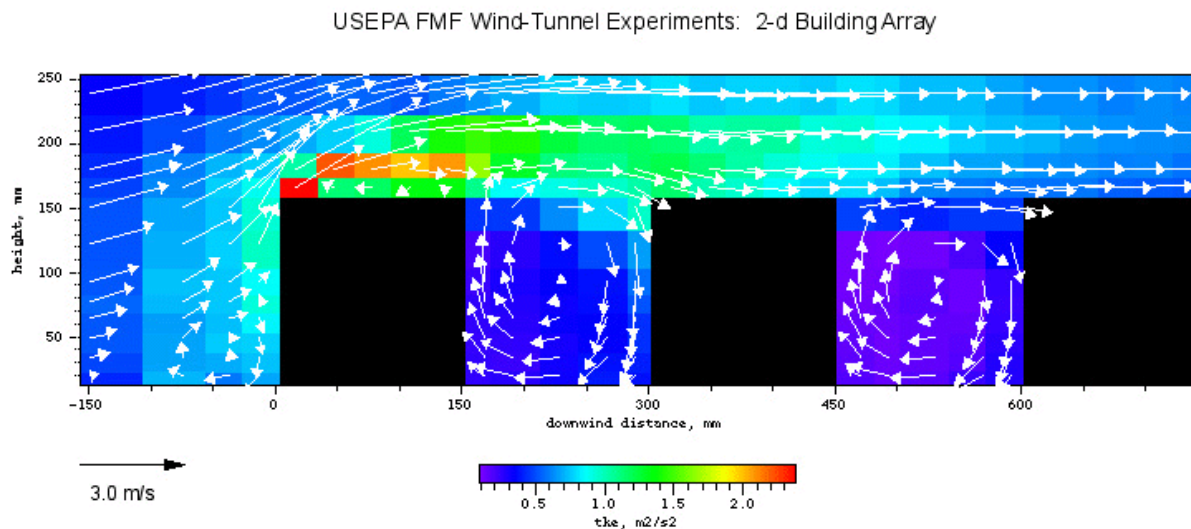
#### **2.4.5 Wind Tunnel Measurements of Mean Flow and Turbulence in an Array of Two-Dimensional Buildings**

A laboratory study of the complex flow patterns within an array of two-dimensional buildings simulating the flows that might be found in a cross-street flow over a number of blocks in an urban area was conducted in the meteorological wind tunnel at the FMF. Aside from using the study data for improving the understanding of the fundamental physics of airflow in urban environments, FMF collaborated with Los Alamos National Laboratory, Los Alamos, New Mexico, and Lawrence Livermore National Laboratory, Livermore, California, to utilize the study data for improving computational fluid dynamics models of flow and dispersion in urban and industrial areas. Previous annual report entries (Poole-Kober and Viebrock, 1999) describing this long-term project have discussed a series of flow visualizations and surface pressure measurements on the buildings. Here the focus is on the mean velocity and turbulence measurements.

Each of the seven buildings, with height (H) and downwind dimension equal to 15 cm, spanned the width of the tunnel. The buildings were each separated in the downwind direction by one building height. High resolution measurements of the three components of mean and turbulent velocities were obtained around and above the array of seven two-dimensional buildings. Although the literature contains descriptions of a fairly abundant number of flow and tracer experiments performed around single buildings (*e.g.*, Meroney, 1982; Hosker, 1984; Lee *et al.*, 1991; and Snyder and Lawson, 1994), relatively few wind tunnel measurements of mean flow

and turbulence intensities within the street canyons and above the buildings have been carried out for multi-building arrays (*e.g.*, Roth and Ueda, 1998; Davidson *et al.*, 1996). This study was designed to supplement these limited studies with high density measurements of mean flow and turbulent kinetic energy.

The approach flow to the building array was a simulated neutral atmospheric boundary layer of a depth of approximately  $12 H$  with sufficient upwind fetch to grow to equilibrium before reaching the upwind edge of the buildings. The approach flow at  $z = H$  was  $3 \text{ m/s}$  ensuring that Reynolds number independence was satisfied. Measurements of the three component velocities and the turbulence intensities were obtained with pulsed-wire anemometry (Bradbury and Castro, 1971). Measurements on the longitudinal centerline of the building array were collected from  $3.5 H$  upstream to  $7.5 H$  downstream of the building arrays and up to  $3 H$  in the vertical. Figure 3 shows the mean wind vectors and the turbulent kinetic energy (tke) around and upstream of the first three buildings. Close inspection reveals a rotor that forms on the upwind face of the first building. More obvious are the single large vortices that form within each building canyon. Of particular interest is the separation zone and reverse flow that forms on the rooftop of the first building but not on subsequent rooftops. This agrees with smoke visualization studies and those of Meroney *et al.* (1996). Additionally, the streamlines above and just upwind of the leading edge of the second building are descending slightly, resulting in stronger downward motion in the first canyon vortex circulation compared to those in subsequent canyon circulations. Figure 3 also shows a large tke maximum at the leading edge of the first building's rooftop and an envelope of large tke values extending above the first two buildings but dying out quickly with downwind distance. The region of highest turbulence above the first building is correlated with a region of strong shear in the flow.



**Figure 3.** Wind vector and turbulent kinetic energy fields measured along the centerline of an array of buildings. The first three of seven buildings are shown here.

## 2.4.6 Meteorological Measurements

Local meteorology is a key factor in both diurnal and day-to-day changes in the ambient pollution concentration levels affecting human exposure. Routine meteorological models can provide gridded data for the entire United States, but the resolution of the grid is not always sufficient for determining local meteorology in support of human exposure modeling. Similarly, routine meteorology measured at airports or other stations is only representative of the surrounding area. The Meteorological Instrumentation Cluster of 3 Trailers (MIC3) is being used to support site specific field studies of human exposure to better identify meteorological factors related to human exposure to air pollutants. The three trailers presently include (See Figure 4):

- AV Model 2000 SODAR<sup>19</sup>:  
Wind (3D) measurements from 60 m to 600 m (30 m intervals, 10 minute average).  
Portable but AC connection required.
- AV Model 4000 miniSODAR:  
Wind (3D) measurements from 15 m to 200 m (5 m intervals, 5 minute average).  
Portable with battery operation for 3-4 days (or AC continuous).
- 10 Meter Tower:  
Wind (2D) measurements at 2, 5, and 10 m (5 minute average).  
Temperature and humidity measurements at 2 and 10 m (5 minute average).

In addition, these measurements of local meteorology near the surface will be used to develop and evaluate a local scale meteorological modeling system for general application in support of human exposure modeling. Measurements may be retrievable in real time. Cooperative research is ongoing with the North Carolina Climate Office, Raleigh, North Carolina, in examining local meteorology models, including CALMET diagnostic model and the ARPS (Advanced Regional Prediction System) forecast model supported by measurements from the MIC3 as well as measurements at Raleigh-Durham Airport, Morrisville, North Carolina, and four other surface 10 m towers. Pilot studies are ongoing in the Research Triangle Park, North Carolina area. MIC3 started collecting data within the Research Triangle Park area when the equipment became operational in March 2000. Figures 5 and 6 display measurements observed for a typical clear summer day. Figure 5a displays the digital facsimile analysis (DFS) from the Model 2000 SODAR. After midnight the temperature difference corresponds to a slightly stable surface layer. The DFS data place the stable boundary layer below 100 meters. After sunrise at 0800 LT, the static stability becomes unstable in response to surface heating. Late afternoon around 1800 LT the static stability becomes stable once again. At this point, the boundary layer quickly collapses to about 130 meters. It is worth noting that some echoes remain above the boundary layer after sunset. These are believed to be due to diminishing turbulence in the

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<sup>19</sup>SODAR: Sound Detection And Ranging



**Figure 4.** The Meteorological Instrumentation Cluster of 3 Trailers used to support field studies of human exposure to air pollutants.

residual layer. Tower wind speed measurements, shown in Figure 5b, have periodic variation throughout the day. Qualitatively, it appears that the sharp changes in wind speed may be related to the convective thermals. Wind speed diminishes near sunset, when the boundary layer collapses (1800 LT).

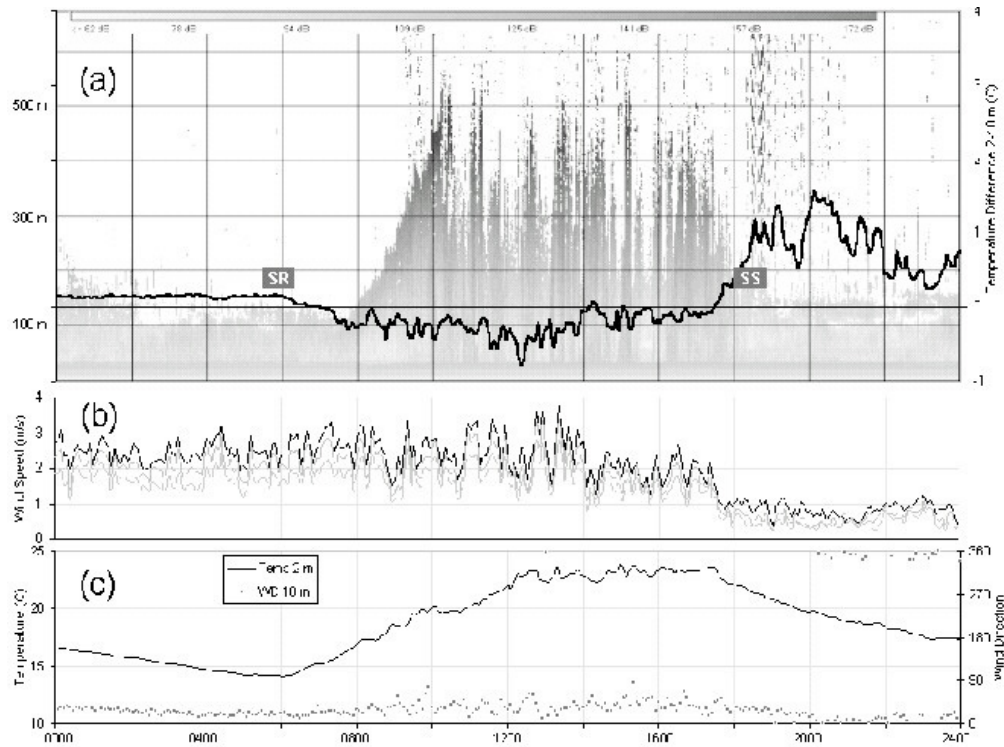
The miniSODAR vertical wind speed profile is shown in Figure 6. During stable conditions, light winds at the surface increase quickly with height to the top of the stable boundary layer (SBL). It is noticed that a wind speed maximum exists (nocturnal jet) near where the DFS analysis places the SBL height (100 meters). During boundary layer growth this momentum is quickly mixed and the wind speed becomes nearly constant with height. When the boundary layer collapses during the late afternoon, the wind speed becomes light near the surface increasing again with height to the top of the SBL where another nocturnal jet is formed (130 meters).

#### **2.4.7 Local Scale Modeling of Human Exposure Microenvironments**

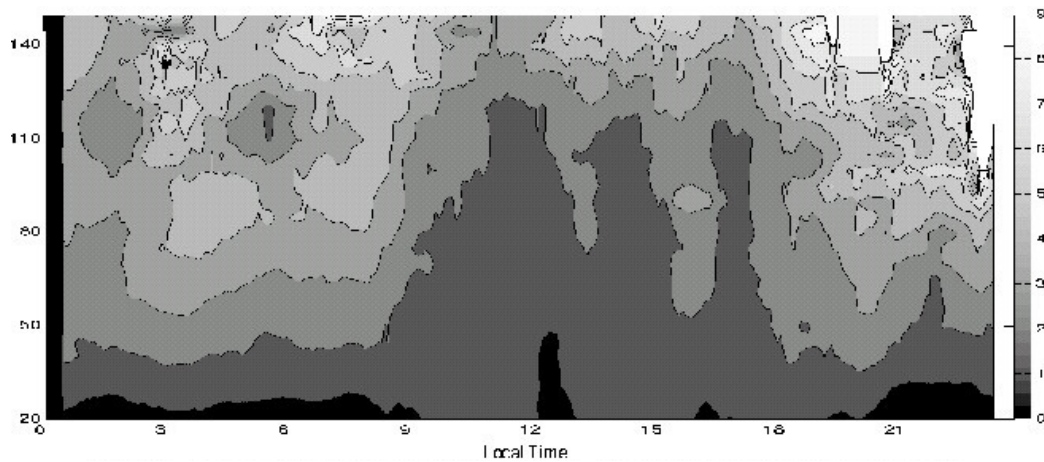
A project to specifically improve the methodology for real-time site specific modeling of human exposure to motor vehicle emissions is ongoing. This project is being pursued in collaboration with other projects by EPA. The goal is to develop improved methods for modeling air pollution from the source through the air pathway to human exposure in significant microenvironments. Local-scale modeling refers to spatial scales from the size of an individual vehicle to the order of 1 km. A complete modeling framework from source-to-exposure together with some measurements is principally being set up in the Research Triangle Park area of North Carolina, which can be transferred to other locations. Human exposure models use simplified assumptions based on a few fixed air monitoring stations or modeled concentrations from regional-scale motor vehicle emission/transport models resulting in great uncertainty in their estimations.

The first component of the modeling framework is real-time site-specific motor vehicle emission models capable of capturing real-world emissions. Development of a real-time **Microscale automobile emission Factor model for Carbon Monoxide (MicroFacCO)** was completed (Singh and Huber, 2000). Performance evaluation studies of MicroFacCO are ongoing. Development of a particulate matter version should be completed during 2001. This work demonstrates the application and sensitivity of emission estimates from these models to real-time input parameters for vehicle fleet composition, vehicle speed, and meteorological conditions. The emission rates calculated from these models can be used in conjunction with a roadway air dispersion model to estimate the ambient concentrations near roadways for a range of traffic fleet and meteorological conditions.





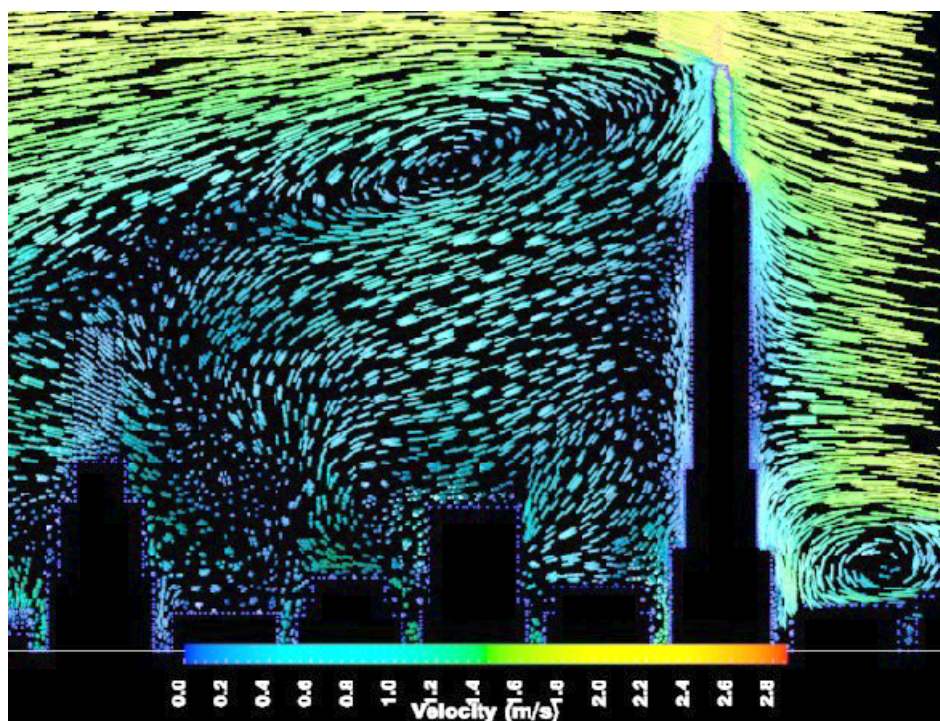
**Figure 5.** (a) Digital facsimile profile from the Model 2000 SODAR and temperature gradient between 2 and 10 meters on September 8, 2000. Sunrise (SR) and sunset (SS) are indicated. (b) Tower measured wind speed at 2, 5, and 10 meters. (c) Temperature at 2 meters and wind direction measured at 10 meters.



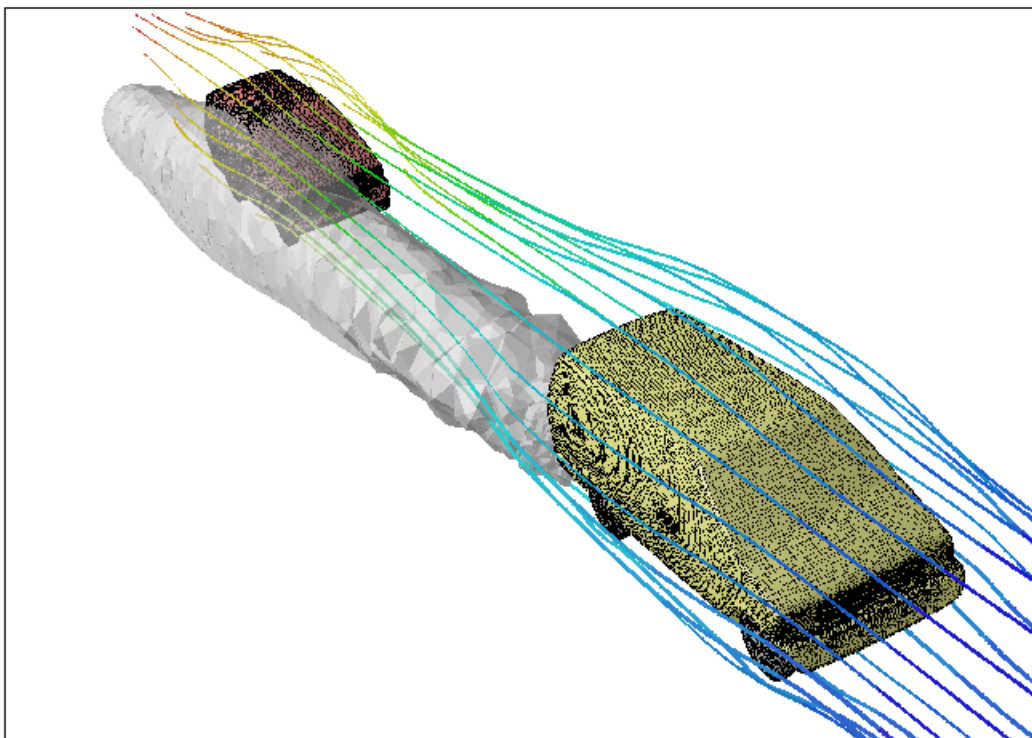
**Figure 6.** Diurnal wind speed profile from the Model 4000 miniSODAR on September 8, 2000. Wind speed is smoothed with a 1-hour moving window. Legend to the right is in meters per second and height on the left is in meters.

The second component will be a local-scale meteorological and air dispersion model to provide ambient air concentrations resulting from transport and other human activities. Refined modeling using Computational Fluid Dynamics (CFD) simulations and measurements are being applied to develop refined air dispersion models for linkage to a roadway microenvironmental model. This modeling framework will help to establish the direct relationships between source-to-exposure concentrations specific to the particular exposure microenvironment (*e.g.*, standing by the roadside or actually inside the vehicle, inside the moving vehicle, living nearby a roadway). Output from this deterministic modeling of microenvironmental concentrations and measured microenvironmental concentrations for a range of scenarios will be used to develop distributions of potential exposure that is probabilistically-based to support population-based human exposure modeling.

Figures 7 and 8 provide two examples of CFD simulation models that were set up for evaluation. CFD simulations provide opportunities for expanding and improving capabilities for modeling exposures to environmental pollutants. A cooperative research project with Fluent, Inc., is examining and evaluating the application of CFD models for simulating air pollution along the pathway from source to human exposures. The detailed spatial resolution of environmental pollution concentrations that is possible from CFD simulations can provide important information that is not available from a single point measurement. Output of CFD simulations can be used to develop better simplified modeling methods in the same way as field and wind tunnel study measurements are used. Through further research, validation and testing, CFD modeling has the potential to become a reliable tool for estimating pollutant concentrations for situations that today have no reliable modeling method.



**Figure 7.** Example of simulation of the wind over Manhattan.



**Figure 8.** Example of CFD simulation of airflow between two moving vehicles and consequences of leading vehicle tailpipe emission.

## 2.5 Air Policy Support Branch

The Air Policy Support Branch supports the activities of the EPA Office of Air Quality Planning and Standards (OAQPS). The Branch responsibilities include evaluating, modifying, and improving atmospheric dispersion and related models to ensure adequacy, appropriateness, and consistency with established scientific principles and Agency policy; preparing guidance on evaluating models and simulation techniques that are used to assess, develop, or revise national, state, and local pollution control strategies for attainment and maintenance of National Ambient Air Quality Standards (NAAQS); and providing meteorological assistance and consultation to support OAQPS in developing and enforcing Federal regulations and standards and assisting the EPA Regional Offices.

## 2.5.1 Modeling Studies

### 2.5.1.1 Air Quality Assessment of Heavy-Duty Engine/Vehicle and Highway Diesel Fuel Rulemaking

Section 202(a)(3) of the Clean Air Act (CAA) requires EPA to set standards for heavy-duty trucks that reflect the greatest degree of emission reduction achievable through available technology. Section 211(c) of CAA allows EPA to regulate fuels in those instances where the emission products of the fuel significantly impair the performance of any emission control device. Based on these two sections of CAA, EPA proposed new regulations to reduce PM and NO<sub>x</sub> emissions from heavy-duty vehicles.

A substantial air quality modeling analysis was performed in FY-2000 to assess the need for the rulemaking and estimate the benefits of the proposed emission reductions. The modeling was closely patterned after the Tier 2/Low Gasoline Sulfur analyses that were successfully completed in FY-1999. A base-year emission inventory was developed for 1996 and projection-year inventories were created for 2007, 2020, and 2030. The proposed heavy-duty engine (HDE) emission reductions were then applied to the 2020 and 2030 cases. Air quality modeling was performed for six scenarios: the base year, three-future year baseline scenarios, and two future-year control scenarios.

The ozone modeling was conducted using the variable-grid version of the Urban Airshed Model (UAM-V). Ozone was simulated over two large regional domains, one covering the eastern United States from the Plains States to the East Coast, and the other covering the remaining lower 48 states to the West Coast. For the eastern domain, three multi-day periods of high observed ozone during the summer of 1995 were selected for the analyses. The meteorological data used to drive the eastern United States UAM-V modeling were obtained from applications of RAMS. For the western domain, two multi-day periods of high observed ozone during the summer of 1996 were selected for the analyses. The meteorological data used to drive the western United States UAM-V modeling were obtained from applications of MM5. The ozone modeling results were evaluated against existing ambient ozone data to assess the quality of model performance. In general, the eastern United States application featured relatively small values of model bias and error (*i.e.*, less than 10% bias, less than 25% error), whereas the western United States simulations consistently underestimated observed ozone by large amounts with a bias of about 40%. Ultimately, only the eastern United States modeling results were used to justify and quantify the effects of the rulemaking.

The modeling runs indicated that in many metropolitan areas continued exceedances of the ozone NAAQS were possible in the future years of 2007, 2020, and 2030. It was estimated that 35-45 areas in the United States (128 million people) were at risk of exceeding the ozone standard sometime between 2007 and 2030. While the HDE emission reductions would not eliminate all of the projected exceedances in the future, the modeling results indicated that ambient ozone levels would be significantly lowered. In 2020, the domain-wide average daily peak 1-hour ozone value was reduced from 81.0 to 78.2 ppb for the episode days. In 2030, the

average daily peak value was estimated to drop from 83.1 to 79.3 ppb when the HDE fleet is almost fully turned over, but overall emissions are rising.

Simulations to estimate the impacts of the proposed HDE regulations on PM were obtained using the Regulatory Modeling System for Aerosols And Deposition (REMSAD). This model was applied for the 1996 base case and 2030 baseline and control scenarios for the entire year of 1996 at a 36-km resolution. The meteorological data were generated using MM5. The results of these simulations are being analyzed and interpreted to quantify the expected benefits of the HDE NO<sub>x</sub> and PM reductions. The full suite of ozone and PM modeling results will provide the air quality basis for the regulatory impact analysis portion of the HDE rulemaking, which is to be signed by the EPA Administrator by the end of 2000.

#### **2.5.1.2 CMAQ Proof of Concept: Western United States Ozone Modeling**

As part of a proof-of-concept effort designed to more fully understand the details of the Models-3/CMAQ modeling system, Models-3/CMAQ was configured and successfully applied for a July 1996 ozone episode over the western United States. The simulations were completed for a 36- and 12-km nested grid with 12 vertical layers. The meteorological input fields were developed using MM5 and the emissions were based on a version of the national emissions trend inventory.

Several configurations of CMAQ were compiled and executed, and several diagnostic simulations were completed, before a successful base case simulation was achieved. In particular, the modeling applied two different chemical solvers and tested the effects of a plume-in-grid algorithm. One solver (Hertel) was found to be significantly faster than the other solver (QSSA), yet yielded comparable results. Although the faster solver is still being evaluated, it is particularly appealing for large-scale CMAQ applications because of its greater computational efficiency. The CMAQ PinG algorithm was successfully applied for 100 point sources and generated results comparable to other PinG approaches.

A limited model performance evaluation, consisting only of surface ozone comparisons, was conducted for one of the base cases. Underestimations of ozone were prevalent, with a mean bias of about -23 percent. Although CMAQ predictions were relatively accurate in the eastern portions of the domain (*e.g.*, Denver, Albuquerque, and Salt Lake City), they were significantly lower than observations in the urbanized portions of California. Comparisons of CMAQ statistical performance results with those from a past UAM-V application for the same domain and episode showed somewhat better model performance within CMAQ. It is suspected that the causes of the under predictions in both exercises are due to underestimated motor vehicle and biogenic emission inventories. Work is underway to investigate the causes of the under predictions of ozone.



### **2.5.1.3 Statistical Evaluation of Model Performance**

Within the American Society for Testing and Materials (ASTM) a Standard Guide (Z6849Z ) is being developed to provide guidance on construction of objective statistical procedures for comparing air quality simulation modeling results with tracer field data. Thus far, those most involved in the development of this ASTM Guide have been scientists within the European community, where there is still strong interest in short-range plume and puff dispersion models. To focus the discussion, a draft evaluation procedure was constructed that measures how well short-range dispersion models characterize the variation of the centerline maximum concentration at the surface as a function of transport distance and stability. The draft ASTM Guide was circulated for review in July 2000. Editorial changes are being addressed. The Guide will be resubmitted for approval in early 2001.

### **2.5.1.4 The Krakow Urban Air Pollution Project**

Local urban air pollution, including pollution from mobile sources, was recognized by the Environment for Europe Ministerial Conference as an area of high priority for the countries of the region. The EPA and Polish Ministry of Environment made this environmental problem one of six focal points for their cooperation. By focusing on the City of Krakow, this project seeks to build upon five years of cooperation between Poland and the United States. in improving the air quality in the Krakow Metropolitan Area. The Krakow Urban Air Pollution project, under the sponsorship of the U.S. Agency for International Development, will assist local authorities to identify, quantify, and develop mitigation strategies for the control of air pollution in the City of Krakow, primarily from the transportation sector.

This project builds on the EPA Office of International Activities work in the Krakow area, which assisted in the identification, quantification, and dissemination of air pollution information in Krakow, primarily from stationary sources and low-level emitters. At the heart of this project is the task of training local staff to conduct air quality modeling studies. This would allow the local authorities to assess their air pollution problems caused by the increase in mobile source pollution, while establishing a basis for more informed national decision-making through the use of improved data, improved analytical tools, and transportation control options.

Following the initial training course in December 1998, a series of training sessions were scheduled over the following 18 months. This allowed the students to first learn the basics, and then gradually allowed hands-on training in the initial application of the modeling system to characterize pollutant impacts in the Krakow area. In May 2000, a training session was held in Krakow to review the procedures to be used in processing the meteorological data, and to initially review the just completed emission inventories. Based on a series of test runs, the modeling team began to suspect that the home heating sulfur-dioxide emissions appeared to be too high. Refinements in the characterization of land-use (pattern of surface roughness lengths and urban versus rural land-use) and emission characterizations (initial release heights and initial

dilution volumes) were decided upon. A final training session will take place in November 2000, as well as a review of the test runs the students completed over the summer months.

#### **2.5.1.5 Improvements to the Regulatory Modeling System for Aerosols and Deposition**

In coordination with the EPA Office of Water, a review was conducted of REMSAD, and a number of errors and deficiencies in the model and several of the accompanying data sets were identified. The appropriate corrections to the model and data sets were determined and implemented. An MM5 to REMSAD conversion program was developed to provide the interface for using MM5 meteorological outputs to derive the specific meteorological inputs needed to run REMSAD. This interface was run to obtain 1996 36-km meteorological inputs for REMSAD. The 1996 36-km data represented a major scientific improvement to the previous set of meteorological inputs, which were derived from 80-km MM4 runs for 1990.

In addition, several components of the REMSAD emission pre-processor were revised, reducing the time needed to process a set of annual emissions from two weeks to four days. With the model corrections, emission data from the revised processor, and the improved meteorological inputs, REMSAD was used to generate six policy-relevant emission scenarios. This version of REMSAD is being studied by the EPA Integrated Strategies and Economics Group as a quick turnaround PC-based screening tool to provide estimates of PM concentrations in support of cost-benefits analyses.

### **2.5.2 Modeling Guidance**

#### **2.5.2.1 Support Center for Regulatory Air Models**

During FY-2000, several activities were accomplished by the SCRAM (Support Center for Regulatory Air Models) web site manager. An extensive testing and checking operation was developed to ensure that all of the air quality models and programs were Y2K compliant. Changes made involved contract support as well as in-house resources. To make the SCRAM documents more universally accepted by all printers, the documents were converted from WordPerfect to PDF format. For the first time, presentations made at the Regional, State, and Local Modeler's Workshop were provided via SCRAM. Due to potential security breaches, the EPA Enterprise Technology Services Division provided upgraded and more extensive firewalls to prevent security infractions from outside Internet connections. However, there were no security breaches encountered on the SCRAM website. There were a total of 41 activities (new items, updates, revisions, etc.) logged during FY-2000.

### **2.5.2.2 Models-3 Help Desk**

The Models-3 Help Desk is an initiative to provide full-time assistance to Models-3 users, during both installation and model application. Models-3 is a multiscale air quality model that provides modeling in a one-atmosphere environment using a graphical user interface based framework, accounting for such processes as chemistry and aerosol interactions, and providing graphical and tabular output. A formal support network comprises the Help Desk with capable and accessible technical experts knowledgeable in the different modules and scientific processes that are performed within the model. During FY-2000, the Models-3 Help Desk responded to various users from Regional and State environmental offices, Canada, and Great Britain. Two surveys were taken by the Help Desk to gather information on the progress and success of the original Models-3 tape installation and to ascertain the type of system the Models-3 users are using and prefer, along with any problems.

### **2.5.2.3 Ad Hoc Meteorological Modeling Workgroup**

Over the past several years there was an encouraging increase in the amount of discussion among members of the regulatory air quality modeling community. Several ad hoc groups were formed as informal mechanisms for the exchange of knowledge between many of the most active State/Local/Federal modelers. A group focused on air quality modeling tools and databases was formed in 1998 and a group focused on emissions inventory development was formed in 1999. EPA staff identified the need for a separate group that focused on the development of meteorological input for regional air quality models, and with significant help from the community as a whole, formed the Ad Hoc Meteorological Modeling workgroup.

The first meeting of the workgroup was held at the University of Maryland in August 2000. A Branch staff member served as the Chair of the workgroup for FY-2000. It was agreed by the 33 meteorological modelers attending the inaugural meeting that the primary purpose of the group is to foster a community exchange of information related to numerical meteorological modeling for eventual air quality modeling purposes. Furthermore, group members agreed that the workgroup should work closely with the two other ad hoc groups, emission modeling and air quality modeling, to improve the overall practice of air quality modeling.



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## APPENDIX A: ACRONYMS, ABBREVIATIONS, AND DEFINITIONS

ACM	Asymmetric Convective Model
AQM	Air Quality Model
AQMF	Air Quality Modeling Forum
ARL	Air Resources Laboratory, NOAA
ARPS	Advanced Regional Prediction System
ASLI	Atmospheric Science Librarians International
ASMD	Atmospheric Sciences Modeling Division
ASPEN	Assessment System for Population Exposure Nationwide
ASTM	American Society for Testing and Materials
AVHRR	Advanced Very High Resolution Radiometer
AVIRIS	Airborne Visible and Infrared Imaging Spectrometer
BASC	Board on Atmospheric Sciences and Climate (NRC/NAS)
BCON	Boundary CONditions processor
BEIS	Biogenic Emissions Inventory System
$b_{\text{ext}}$	Extinction coefficient
CAA	Clean Air Act of 1970
CAAA	Clean Air Act Amendments of 1990
CAPITA	Center for Air Pollution Impacts and Trends Analysis
CASTNet	Clean Air Status and Trends Network
CB-IV	Carbon Bond-IV
CBL	Convective Boundary Layer
CCTM	CMAQ Chemistry-Transport Model
CD-ROM	Compact Disk - Read Only Memory
CFD	Computational Fluid Dynamics
CMAQ	Community Multiscale Air Quality model
CTM	Chemistry-Transport Model
DFS	Digital Facsimile Analysis
DIAS	Dynamic Information Architecture System
ECIP	Emissions-Chemistry Interface Processor
EDAS	Eta Data Assimilation System
EMEP	European Monitoring and Evaluation Programme
EPA	Environmental Protection Agency
Extended RADM	Regional Acid Deposition Model with full dynamics of secondary inorganic fine particle formation taken from the RPM
FAMS	Florida Atmospheric Mercury Study
FCMSSR	Federal Committee for Meteorological Services and Supporting Research
FDDA	Four-Dimensional Data Assimilation
FMF	Fluid Modeling Facility (EPA)
FTP	File Transfer Protocol
FY	Fiscal Year
GIS	Geographic Information System



HDE	Heavy Duty Engine
HPCC	High Performance Computing and Communications
HTML	HyperText Markup Language
IAMSLIC	International Association of Aquatic and Marine Science Libraries and Information Centers
ICMSSR	Interdepartmental Committee for Meteorological Services and Supporting Research
ICON	Initial CONditions processor
I/O	Input/Output
ITM	International Technical Meeting
ITR&D	Information Technology Research and Development
JPROC	Photolysis rate processor
LULC	Land Use/Land Cover
MCIP	Meteorology-Chemistry Interface Processor
MEPPS	Models-3 Emission Processing and Projection System
MIC3	Meteorological Instrumentation Cluster of 3 trailers
MicroFacCO	Microscale automobile emission Factor model for carbon monoxide
MIMS	Multimedia Integrated Modeling System
MIRAGE	Megacity Impact on Regional And Global Environments
MLBC	Multi-Layer Bio-Chemical dry deposition model
MM5	Mesoscale Model - Version 5
Models-3	Third generation air quality modeling system
MODTRAN	MODerate resolution TRANSmittance
MSC-East	Meteorological Synthesizing Center - East
NAAQS	National Ambient Air Quality Standards
NAPAP	National Acid Precipitation Assessment Program
NARSTO	North American Research Strategy for Tropospheric Ozone
NARSTO-NE	NARSTO-NorthEast
NAS	National Academy of Sciences
NASA	National Aeronautics and Space Administration
NATO/CCMS	North Atlantic Treaty Organization Committee on the Challenges of Modern Society
NCAR	National Center for Atmospheric Research
NCEP	National Centers for Environmental Prediction
NERL	National Exposure Research Laboratory
NET	National Emissions Trends
NEXRAD	NEXt generation RADar
NOAA	National Oceanic and Atmospheric Administration
NPS	National Park Service
NSF	National Science Foundation
NWS	National Weather Service
OAQPS	Office of Air Quality Planning and Standards (EPA)
OMB	Office of Management and Budget
PAVE	Package for Analysis and Visualization

PBL	Planetary Boundary Layer
PC	Personal Computer
PDM	Plume Dynamics Model
PEM	Pesticide Emissions Model
PinG	Plume-in-Grid algorithm
PM	Particulate Matter
PPM	Piecewise Parabolic Model
PSU	Pennsylvania State University
PX LSM	Land-Surface Model
QA/QC	Quality Assurance/Quality Control
QSSC	Quality Systems Science Center
R&DF	Research and Development Forum
RADM	Regional Acid Deposition Model
RADM/RPM	Regional Acid Deposition Model/Regional Particulate Model
RAMS	Regional Atmospheric Modeling System
RELMAP	REgional Lagrangian Model of Air Pollution
REMSAD	Regulatory Modeling System for Aerosols And Deposition
RGM	Reactive Gaseous Mercury
RHESSys	Regional Hydro-Ecological Simulation System
RHR	Regional Haze Rule
RPM	Regional Particulate Model
SAEWG	Standing Air Emission Work Group
SAIL	Southeast Affiliate of IAMSLIC Librarians
SASWG	Standing Air Simulation Work Group
SBL	Stable Boundary Layer
SCRAM	Support Center for Regulatory Air Models
SGI	Silicon Graphics Incorporated computing platform
SIP	State Implementation Plan
SMOKE	Sparse Matrix Operator Kernel Emission
SODAR	SOund Detection And Ranging
SoFAMMS	South Florida Atmospheric Mercury Monitoring Study
SOS	Southern Oxidants Study
SWOOMS	Surface Water Object-Oriented Modeling System
TOMS	Total Ozone Mapping Spectrometer
UAM-V	Urban Airshed Model - Variable grid
URL	Uniform Resource Locator
URMM	Urban-Regional Multiscale Model
USGS	U.S. Geological Survey
Vis5D	Visualizing five dimensional gridded data sets
WRAP	Western Regional Air Partnership
WSR-88D	Weather Surveillance Radar 1988 Doppler Version
WWW	World-Wide Web

## APPENDIX B: PUBLICATIONS

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## **APPENDIX C: PRESENTATIONS**

- Benjey, W.G. Experience with Models-3 emission (with and without the framework). Presentation at the First Models-3 Workshop, Washington, DC, June 13, 2000.
- Binkowski, F.S. CMAQ aerosol component. Presentation at Colorado State University, Ft. Collins, CO, March 9, 2000.
- Binkowski, F.S. Evaluation of predicted visual range using the Community Multiscale Air Quality modeling system. Presentation at the European Aerosol Conference, Dublin, Ireland, September 3, 2000.
- Bullock, O.R., Jr. Atmospheric mercury modeling - Investigation of a global pollutant. Presentation at the International Transport of Air Pollutants (ITAP) group meeting, Washington, DC (electronic presentation by conference call from Research Triangle Park, NC), June 27, 2000.
- Bullock, O.R., Jr. Overview of atmospheric mercury modeling at NERL. Presentation at the Ozone/Air Toxics Program Peer Review, Research Triangle Park, NC, June 28, 2000.
- Byun, D.W. One-atmosphere modeling concept: Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Presentation at Arizona State University, Phoenix, AZ, November 10, 1999.
- Byun, D.W. EPA's Models-3/CMAQ. Presentation at National Institute for Environmental Studies, Tsukuba, Japan, February 5, 2000.
- Byun, D.W. One-atmosphere dynamics in Models-3/CMAQ. Presentation at the Institute for Mathematics and Its Applications Workshop: Atmospheric Modeling, University of Minnesota, Minneapolis, MN, March 16, 2000.
- Byun, D.W. Trans-Pacific modeling - Investigation of a global pollutant. Presentation at the International Transport of Air Pollutants (ITAP) group meeting, Washington, DC (electronic presentation by conference call from Research Triangle Park, NC), June 27, 2000.
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- Ching, J.K.S. Air quality and exposure modeling: Potential and implementation for their linkage. Presentation at the Workshop on the Implementation of Long Term Exposure to PM for Epidemiology Studies, Research Triangle Park, NC, December 6, 1999.
- Ching, J.K.S. Mathematical and modeling issues: EPA's Models-3/CMAQ modeling system. Presentation at the Air Quality Seminar for the University of Houston, Department of Mathematics, Houston, TX, April 27, 2000.
- Cooter, E.J. Atmospheric transport and deposition of atrazine to Lake Michigan. Presentation at the Lake Michigan Mass Balance Study Atrazine Modeling Peer Review Meeting, Romulus, Michigan, September 27, 2000.
- Dennis, R.L. Evaluating complex and/or multi-disciplinary models: The difficulty necessitates new, more diagnostic approaches. Presentation at the SETAC 20th Annual Meeting, Philadelphia, PA, November 15, 1999.
- Dennis, R.L. Atmospheric deposition of nutrients to coastal waters. Presentation at the SETAC 20th Annual Meeting, Philadelphia, PA, November 17, 1999.
- Dennis, R.L. EPA's third generation air quality model and modeling system: Models-3/CMAQ, a one-atmosphere approach. Presentation at the National Center for Atmospheric Research, Boulder, CO, December 7, 1999.
- Dennis, R.L. NO<sub>x</sub>: A one-atmosphere perspective. Presentation on the EPA Office of Air Quality Planning and Standards NO<sub>x</sub> Telecast, Raleigh, NC, December 8, 1999.
- Dennis, R.L. Atmospheric deposition of nutrients to coastal waters of the East and Gulf Coasts: From where does it originate - sources and airsheds. Presentation at the SAIL 2000 Conference, Research Triangle Park, NC, April 5, 2000.
- Dennis, R.L. Regional air quality modeling perspective. Presentation at the EPA Dry Deposition Workshop, Washington, DC, May 24, 2000.
- Dennis, R.L. Characterization of principal airsheds of atmospheric deposition of nutrients to East and Gulf Coast estuarine watersheds. Presentation at the American Geophysical Union Spring 2000 Meeting, Washington, DC, June 1, 2000.
- Dennis, R.L. Principal airsheds of sulfur and oxidized nitrogen deposition to Shenandoah National Park. Presentation at the American Geophysical Union Spring 2000 Meeting, Washington, DC, June 2, 2000.
- Dennis, R.L. First results from testing the operational performance of the EPA Community Multiscale Air Quality model (CMAQ). Presentation at the First Annual Models-3 Workshop, Arlington, VA, June 12, 2000.

- Dennis, R.L. Atmospheric transport and airsheds for Neuse/Pamlico System. Presentation at the EPA MIMS Workshop, Research Triangle Park, NC, August 15, 2000.
- Dennis, R.L. Atmospheric deposition of inorganic nitrogen to watersheds/estuarine waters. Presentation at the Cross Discipline Ecosystem Modeling and Analysis Workshop, Research Triangle Park, NC, August 16, 2000.
- Dolwick, P.D. CMAQ proof of concept: Western United States ozone modeling. Presentation at the First Annual Models-3 Workshop, Arlington, VA, June 12, 2000.
- Dolwick, P.D. U.S. EPA plans for meteorological modeling in FY-2001: CMAQ proof of concept — Eastern United States fine grid ozone/PM modeling for July 1995. Presentation at the Ad Hoc Meteorological Modeling Workgroup, College Park, MD, August 16, 2000.
- Eder, B.K. An aggregation and episode selection scheme for EPA's Models-3 CMAQ. Presentation at the Environmental Statistics Seminar Series at North Carolina State University, Raleigh, NC, April 20, 2000.
- Eder, B.K. A Preliminary Evaluation of Models-3 CMAQ Using Visibility Parameters. Presentation at the 14<sup>th</sup> Annual International Symposium on the Measurement of Toxic and Related Air Pollutants, Research Triangle Park, NC, September 13, 2000.
- Fine, S.S. Status of MIMS architecture design. Presentation at Cross-Discipline Ecosystem Modeling and Analysis Workshop, Research Triangle Park, NC, August 16, 2000.
- Fine, S.S. A framework for creating and managing graphical analyses. Presentation at Cross-Discipline Ecosystem Modeling and Analysis Workshop, Research Triangle Park, NC, August 17, 2000.
- Fine, S.S. Multimedia Integrated Modeling System update. Presentation at Council on Regulatory Environmental Modeling, Washington, DC, September 7, 2000.
- Gillette, D.A. K factor comparisons with Fa/q. Presentation at the Review of Preliminary Findings of the Owens Lake Dust ID Project, Bishop, CA, June 15, 2000.
- Gilliland, A.B. Introduction: MIMS ecosystem modeling integration efforts. Presentation at the Cross-Discipline Ecosystem Modeling and Analysis Workshop, Research Triangle Park, NC, August 15, 2000.
- Lawson, R.E., Jr., R.S. Thompson, S.G. Perry, and W.H. Snyder. Modeling puff diffusion in a laboratory convection tank. Presentation at the 11<sup>th</sup> Joint Conference on the Applications of Air Pollution Meteorology with the A&WMA, Long Beach, CA, January 10, 2000.

LeDuc, S.K. Lightning safety. Presentation to two Kindergarten classes at Sangamon Elementary School, Mahomet, IL, October 21, 1999.

LeDuc, S.K. Lightning safety. Presentation to two 4<sup>th</sup> grade classes at Lincoln Trail Elementary School, Mahomet, IL, October 21, 1999.

LeDuc, S.K. Lightning safety. Presentation to three 1<sup>st</sup> grade classes at Memorial Elementary School, Paris, IL, October 22, 1999.

LeDuc, S.K. An overview of Models-3/CMAQ. Presentation to the Air Pollution Training Institutes Satellite Broadcast, Research Triangle Park, NC, December 9, 1999.

LeDuc, S.K. An overview of Models-3/CMAQ. Presentation to the Mid-Atlantic Region Air Managers Association, Wilmington, DE, January 12, 2000.

LeDuc, S.K. Expanding your horizons weather jeopardy. Presentation to an audience of 7<sup>th</sup> grade girls at North Carolina State University, Raleigh, NC, March 14, 2000.

Otte, T.L. Lightning. Presentation to four 5<sup>th</sup> grade classes at Zebulon Elementary School, Zebulon, NC, December 3, 1999.

Otte, T.L. Evaporation and condensation. Presentation to five 2<sup>nd</sup> grade classes, Smith Elementary School, Raleigh, NC, December 17, 1999.

Otte, T.L. Careers in meteorology (3 sessions). Presentation at Carroll Middle School, Raleigh, NC, March 24, 2000.

Otte, T.L. Evaporation and condensation (3 sessions). Presentation to the 2<sup>nd</sup> grade at West Lake Elementary School, Apex, NC, April 7, 2000.

Otte, T.L. Evaporation and condensation (4 sessions). Presentation to the 2<sup>nd</sup> grade at Willow Springs Elementary School, Willow Springs, NC, May 5, 2000.

Otte, T.L. Using Eta model analyses to initialize MM5 v3. (Brown bag seminar). Presentation to AMDB, Research Triangle Park, NC, May 25, 2000.

Otte, T.L. MM5: A community prototype for CMAS. Presentation at the First Annual Models-3 Workshop, Arlington, VA, June 13, 2000.

Otte, T.L., and S.K. LeDuc. Weather jeopardy (2 sessions). Presentation at 8th Expanding Your Horizons Workshop, North Carolina State University, Raleigh, NC, March 14, 2000.

Perry, S.G. Overview of AERMOD dispersion model. Presentation to the Neighborhood Scales Working Group, Research Triangle Park, NC, June 1, 2000.

- Pierce, T.E. Winter storms. Presentation at Durant Elementary School, Raleigh, NC, December 20, 1999.
- Pierce, T.E. The importance of lightning and other natural sources of NO<sub>x</sub> and VOCs for regional air quality modeling. Invited presentation at the Universities Space Research Association, Huntsville, AL, October 20, 1999.
- Pierce, T.E. Overview of the OZark Isoprene Experiment (OZIE). Presentation at the Fall Meeting of the American Geophysical Union, San Francisco, CA, December 14, 1999.
- Pierce, T.E. Advances in biogenic emissions modeling. Invited presentation at the California Air Resources Board's Workshop on Biogenic Emissions Research, Sacramento, CA, December 9, 1999.
- Pierce, T.E. Issues regarding isoprene emissions for ozone model simulations. Presentation at the Ad Hoc Emission Modeling Workshop, Baltimore, MD, January 20, 2000.
- Pierce, T.E. The evolution of biogenic emission inventory modeling systems for regional air quality modeling. Invited presentation at the Gordon Research Conference on Biogenic VOCs and the Atmosphere, Ventura, CA, March 2, 2000.
- Pierce, T.E. The role of agriculture on airborne nitrogen emissions. Presentation at the Ammonia Emission Modeling Workshop, Beltsville, MD, March 22, 2000.
- Pierce, T.E. Development of a 1-km vegetation database for modeling biogenic fluxes of hydrocarbons and nitric oxide, Sixth International Conference on Air-Surface Exchange of Gases and Particles, Edinburgh, United Kingdom, July 3, 2000.
- Pierce, T.E. Development of a 1-km vegetation cover database. Presentation at the Cross-Discipline Ecosystem Modeling and Analysis Workshop, Research Triangle Park, NC, August 17, 2000.
- Pleim, J.E. Dry deposition modeling in the Models-3 Community Multiscale Air Quality (CMAQ) model system. Presentation at the Workshop on Dry Deposition in North America, Washington, DC, May 22, 2000.
- Pleim, J.E. A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes. Presentation at the 6th International Conference on Air-Surface Exchange of Gases and Particles in Edinburgh, Scotland, July 5, 2000.
- Poole-Kober, E.M. Atmospheric Science Librarians International. Poster presentation at the 25<sup>th</sup> IAMSLIC Annual Conference, Woods Hole, MA, October 20, 1999.

- Poole-Kober, E.M. Field study experience at the Atmospheric Sciences Modeling Division. Spring Field Experience Reception, Student Chapter of the Special Library Association, University of North Carolina at Chapel Hill, Chapel Hill, NC, April 13, 2000.
- Schere, K.L. Status and applications of Models-3/CMAQ. Presentation at US/German Ozone, Fine Particle Science and Environmental Chamber Workshop, Riverside, CA, October 5, 1999.
- Schere, K.L. Models-3/CMAQ - The future of air quality modeling. Presentation at the Conference on Transportation Planning and Air Quality, Lake Lanier, GA, November 17, 1999.
- Schere, K.L. CMAQ model overview. Presentation for the satellite broadcast course on Nitrogen Compounds and Air Quality in the Troposphere, Raleigh, NC, December 9, 1999.
- Schere, K.L. Recent developments in air quality modeling. Presentation at the Conference on Environmental Monitoring, Evaluation, and Protection in New York: Linking Science and Policy, Albany, NY, December 8, 1999.
- Schere, K.L. Models-3/CMAQ and the community modeling concept. Presentation to the CENR-Air Quality Research Subcommittee in Washington, DC, February 18, 2000.
- Schere, K.L. Briefing on Models-3/CMAQ. Presentation to the Administrator, OAQPS, Durham, NC, March 29, 2000.
- Schere, K.L. Regional/urban air quality modeling with U.S. EPA's Models-3/CMAQ. Presentation at Harvard University, Department of Earth and Planetary Sciences, Cambridge, MA, April 7, 2000.
- Schere, K.L. Use of PM data in model evaluation. Presentation at the Eastern Supersites Meeting, Baltimore, MD, April 12, 2000.
- Schere, K.L. Urban/regional air quality modeling with U.S. EPA's Models-3/CMAQ. Presentation at the National Research Council, Committee on Atmospheric Chemistry, Washington, DC, May 11, 2000.
- Schere, K.L. Regional/urban tropospheric air quality modeling with U.S. EPA's Models-3/CMAQ. Presentation at the University of Alabama - Huntsville, Huntsville, AL, May 31, 2000.
- Schere, K.L. U.S. EPA Models-3/CMAQ: What's New in 2000? Presentation at the First Annual Models-3 Workshop, Arlington, VA, June 12, 2000.

- Schere, K.L. Models-3/CMAQ: A system for air quality modeling. Presentation at the Air Quality and Environmental Forecasting Workshop, Silver Spring, MD, June 15, 2000.
- Schere, K.L. Status of the Models-3/CMAQ modeling system. Presentation at the NARSTO Reactivity Research Work Group Meeting, Research Triangle Park, NC, June 30, 2000.
- Schiermeier, F.A. Demonstration of the Supercomputing Center and Scientific Visualization Laboratory. Presentation for the EPA/OEI Assistant Administrator, Research Triangle Park, NC, October 19, 1999.
- Schiermeier, F.A. Demonstration of the Supercomputing Center and Scientific Visualization Laboratory. Presentation for the Environmental Counselor of The Netherlands Embassy and the Director of RIVM in The Netherlands, Research Triangle Park, NC, March 15, 2000.
- Schiermeier, F.A. Past history and future plans for International Technical Meetings on Air Pollution Modeling and Its Application. Presentation at the NATO/CCMS Plenary Meeting of Partner and Alliance Countries, Brussels, Belgium, March 21, 2000.
- Schiermeier, F.A. Great Waters and regional deposition applications. Presentation at the Standing Air Simulation Work Group Meeting, Asheville, NC, April 1, 2000.
- Schiermeier, F.A. Examples of AMD outreach activities. Presentation at the NERL Mid-Year Review by the EPA/ORD Assistant Administrator and the EPA/ORD Deputy Assistant Administrators, Research Triangle Park, NC, April 5, 2000.
- Schiermeier, F.A. Conference Chairman opening address, closing address, and banquet award conferrals. Presentations at the Millennium (24th) NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Boulder, CO, May 15-19, 2000.
- Schiermeier, F.A. Past history and future plans for International Technical Meetings on Air Pollution Modeling and Its Application. Presentation at the Millennium (24th) NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application, Boulder, CO, May 19, 2000.
- Schiermeier, F.A. Demonstration of the Supercomputing Center and Scientific Visualization Laboratory. Presentation to the EPA/OEI Assistant Administrator and Deputy Assistant Administrator, Research Triangle Park, NC, June 1, 2000.
- Schiermeier, F.A. Perspectives on the probability of success for CMAS (Community Modeling and Analysis System) and next steps. Presentation at the First Annual Models-3 Workshop, Arlington, VA, June 14, 2000.



Schiermeier, F.A. Demonstration of the Supercomputing Center and Scientific Visualization Laboratory. Presentation for the EPA/OAR and EPA/OEI Assistant Administrators, Research Triangle Park, NC, September 11, 2000.

Schiermeier, F.A. Contractual support required for the Atmospheric Modeling Division's research programs. Presentation at the Meeting on Federal Dollar\$ and Sense for Women Owned Businesses, U.S. Small Business Administration, Research Triangle Park, NC, September 19, 2000.

Schiermeier, F.A. Overview of the EPA/ORD atmospheric research programs. Presentation to the ICMSSR Committee for Agency Cooperative Research, Washington, DC, September 21, 2000.

Streicher, J.J.. Modeling acute exposure to solar radiation radiation. Presentation at the American Society for Photobiology Meeting, San Francisco, CA, July 3, 2000.

## **APPENDIX D: WORKSHOPS AND MEETINGS**

US/German O<sub>3</sub>/PM Science and Environmental Chamber Workshop, Riverside, CA, October 4–6, 1999.

K.L. Schere

Workshop: Review of Persistent Organic Pollutants and Heavy Metals under the Convention on Long Range Transboundary Air Pollution (LRTAP), Durham, NC, October 5–7, 1999.

J.K.S. Ching

NARSTO Reactivity Research Work Group, Riverside, CA, October 7, 1999.

K.L. Schere

NARSTO Synthesis Team Meeting, Washington, DC, October 18–20, 1999.

K.L. Schere

Atmospheric Deposition of Toxics - Science & Policy Workshop, Chicago, IL, October 21–22, 1999.

O.R. Bullock, Jr.

Fall 1999 Standing Air Emissions Working Group, Stevenson, WA, October 23–24, 1999.

W.G. Benjey

Texas 2000 Planning Meeting, Houston, TX, November 9–10, 1999.

R.L. Dennis

ASCE Conference on Transportation Planning and Air Quality, Lake Lanier, GA, November 16–17, 1999.

K.L. Schere

UNEP/WMO Workshop on Modeling Heavy Metals and POPs, Geneva, Switzerland, November 16–19, 1999.

O.R. Bullock, Jr.

Models-3/CMAQ for Western Regional Air Partnership (WRAP), Salt Lake City, UT, November 30–December 3, 1999.

J.K.S. Ching

Particulate Matter Workshop, Research Triangle Park, NC, December 6–8, 1999.

D.W. Byun  
J.K.S. Ching

Conference on Environment Monitoring, Evaluation, and Protection in New York: Linking Science and Policy, Albany, NY, December 6–8, 1999.

K.L. Schere

Megacity Impact on Regional and Global Environments (MIRAGE) Meeting with NCAR Modelers, Boulder, CO, December 7, 1999.

R.L. Dennis

Workshop on Biogenic Emissions Research, Sacramento, CA, December 8–9, 1999.

T.E. Pierce

EPA/ORD Mercury Research Strategy Peer Review Workshop, Washington, DC, December 8–9, 1999.

O.R. Bullock, Jr.

Gulf of Mexico Program Office Workshop on Nitrogen Deposition to Gulf Coast Estuaries, Houston, TX, December 8–10, 1999.

R.L. Dennis

Fall Meeting of the American Geophysical Union, San Francisco, CA, December 11–16, 1999.

P.L. Finkelstein  
T.E. Pierce

Third Annual Meeting of the Atmospheric Science Librarians International, Long Beach, CA, January 9–14, 2000.

E.M. Poole-Kober

Workshop on Coupling Multi-Physics Problems in Environmental Simulation, Vicksburg, MS, January 11–12, 2000.

A.B. Gilliland

ASTM D22.11 Subcommittee meeting, Long Beach, CA, January 13, 2000.

J.S. Irwin

RARE Field Project, Ft. Lauderdale, FL, January 15–22, 2000.

O.R. Bullock, Jr.

Ad Hoc Emission Modeling Workshop, Baltimore, MD, January 20–21, 2000.

W.G. Benjey

T.E. Pierce

Technically Advanced Smoke Emissions Tools (TASET) Workshop, Ft. Collins, CO, February 2–4, 2000.

J.K.S. Ching

NARSTO NorthEast Ozone and Particulate Study (NEOPS) Workshop, Wilmington, DE, February 7–9, 2000.

R.L. Dennis

North Carolina Regional Science Bowl, North Carolina Central University, Durham, NC, February 12, 2000.

T.L. Otte

Nitrogen 2001 Planning Workshop, Washington, DC, February 15–16, 2000.

R.L. Dennis

CENR Meeting on Models-3/CMAQ, Washington, DC, February 18, 2000.

R.L. Dennis

K.L. Schere

F.A. Schiermeier

Airborne Visible and InfraRed Spectrometer (AVIRIS) Workshop, Pasadena, CA, February 23–25, 2000.

J.J. Streicher

NARSTO Synthesis Team Writing Workshop at Georgia Institute of Technology in Atlanta, Atlanta, GA, February 23–25, 2000.

K.L. Schere

Gordon Research Conference on Biogenic VOCs and the Atmosphere, Ventura, CA, February 27–March 3, 2000.

T.E. Pierce

Chesapeake Bay Air Subcommittee Meeting, Annapolis, MD, February 29, 2000.

R.L. Dennis

Workshop on Modeling Chemistry in Cloud and Air Quality Models, National Center for Atmospheric Research, Boulder, CO, March 6–8, 2000.

F.S. Binkowski  
S.J. Roselle

Southern Oxidants Study Data Workshop, Research Triangle Park, NC, March 6–10, 2000.

J.R. Arnold	T.L. Otte
D.W. Byun	J.E. Pleim
J.K.S. Ching	K.L. Schere
R.L. Dennis	

NARSTO Executive Steering Committee Meeting, Washington DC, March 8–9, 2000.

J.L. West

Eighth Expanding Your Horizons Workshop, North Carolina State University, Raleigh, NC, March 14, 2000.

S.K. LeDuc  
T.L. Otte

Institute for Mathematics and Its Applications Workshop: Atmospheric Modeling, University of Minnesota, Minneapolis, MN, March 15–19, 2000.

F.S. Binkowski  
D.W. Byun  
J.K.S. Ching  
J.E. Pleim

Ammonia Emission Modeling Workshop, Beltsville, MD, March 21–23, 2000.

W.G. Benjey  
T.E. Pierce

Standing Air Emissions Working Group, Asheville, NC, March 31–April 1, 2000.

W.G. Benjey  
F.A. Schiermeier

Tenth Annual SAIL Conference, Research Triangle Park, NC, April 5–7, 2000.

J.K.S. Ching	J.E. Pleim
R.L. Dennis	E.M. Poole-Kober
P.L. Finkelstein	F.A. Schiermeier
T.L. Otte	

Annual ASTM D22 Committee and Subcommittee Meetings, Toronto, Canada April 11–12, 2000.

J.S. Irwin

EPA Supersites Principal Investigators Meeting, Baltimore MD, April 12–13, 2000.

K.L. Schere  
J.L. West

Shenandoah Assessment Planning Meeting, Shenandoah National Park, VA, April 12–13, 2000.

R.L. Dennis

Mercury Modeling Intercomparison Workshop Atmospheric Mercury Models, Meteorological Synthesizing Center - East, Moscow, Russia, April 13–14, 2000.

O. R. Bullock, Jr.

Mercury Source-Receptor Relationship Expert Panel, Madison, WI, May 22–23, 2000.

O. R. Bullock, Jr.

EPA Dry Deposition Workshop, Washington, DC, May 22–24, 2000.

R.L. Dennis  
P.L. Finkelstein  
M. Fuentes

NARSTO PM Assessment Team Meeting, Washington DC, May 24–26, 2000.

J.L. West

RARE Field Project, 2<sup>nd</sup> Phase, Ft. Lauderdale, FL, June 1–11, 2000.

O.R. Bullock, Jr.

MARAMA-SESARM/Metro 4 Workshop: PM<sub>2.5</sub> Emissions Inventory Workshop, Raleigh, NC, June 5–7, 2000.

W.G. Benjey  
F.S. Binkowski

Research Uses of the UVB Monitoring Network, Albuquerque, NM, June 6–7, 1999.

J.J. Streicher

Workshop on Multiscale Atmospheric Dispersion Modeling, Washington, DC, June 6–8, 2000.

A.H. Huber  
R.E. Lawson, Jr.  
W.B. Petersen

First Annual Models-3 Workshop, Arlington, VA, June 12-14, 2000.

D.A. Atkinson	S.K. LeDuc
W.G. Benjey	J.H. Novak
R.L. Dennis	T.L. Otte
P.D. Dolwick	K.L. Schere
M.L. Evangelista	F.A. Schiermeier

Regional/State Workshop, Arlington, VA June 14–16, 2000.

J.S. Irwin

NOAA/OAR Air Quality and Environmental Forecasting Modeling Workshop, Silver Spring, MD, June 15, 2000.

K.L. Schere

F.A. Schiermeier

Human Exposure Source-to-Dose Modeling Research University Partnership Agreements: 2nd Annual Planning Meeting, Research Triangle Park, NC, June 21, 2000.

J.K.S. Ching

K.L. Schere

Tenth PSU/NCAR Mesoscale Model Users' Workshop, Boulder, CO, June 21–22, 2000.

D.W. Byun

T.L. Otte

J.E. Pleim

First Annual WRF Workshop, Boulder, CO, June 23, 2000.

D.W. Byun

T.L. Otte

PSU/NCAR Mesoscale Modeling System Workgroup, Boulder, CO, June 26–29, 2000.

P.D. Dolwick

Workshop on Combining Environmental Fate and Air Quality Modeling, Research Triangle Park, NC, June 27–29, 2000.

F.S. Binkowski

NARSTO Reactivity Research Work Group Meeting, Research Triangle Park, NC, June 30, 2000.

K.L. Schere



Sixth International Conference on Air-Surface Exchange of Gases and Particles, Edinburgh, United Kingdom, July 3–7, 2000.

P.L. Finkelstein  
T.E. Pierce  
J.E. Pleim  
D.B. Schwede

Fourth Annual George Mason University Transport and Dispersion Modeling Workshop, Fairfax, VA, July 11–12, 2000.

D.W. Byun

Place-Based Decision Support System Workshop, Denver, CO, July 15–17, 2000.

S.S. Fine

First International Workshop on Trans-Pacific Transport of Atmospheric Contaminants, Seattle, WA, July 27–29, 2000.

F.A. Schiermeier

NOAA Air Quality Forecasting and Prediction Workshop, Boulder, CO, August 3–4, 2000.

K.L. Schere

EPA Managing Quality Systems Training Conference, Chicago, IL, August 7–9, 2000.

J.L. West

EPA MIMS Workshop, Research Triangle Park, NC, August 15–17, 2000.

R.L. Dennis	J.H. Novak
S.S. Fine	T.E. Pierce
P.L. Finkelstein	D.B. Schwede
A.B. Gilliland	

Ad Hoc Meteorological Modeling Workgroup, College Park, MD, August 16–17, 2000.

P.D. Dolwick

NARSTO Assessment Workshop, Baltimore, MD, September 18–20, 2000.

R.L. Dennis

NARSTO Model Intercomparison Workshop, Chicago, IL, September 26–27, 2000.

J.R. Arnold  
R.L. Dennis

Cross-Discipline Ecosystem Modeling and Analysis Workshop, Research Triangle Park, NC,  
August 15–17, 2000.

W.G. Benjey	J.H. Novak (co-chair)
D.W. Byun	T.L. Otte
J.K.S. Ching	T.E. Pierce
R.L. Dennis	J.E. Pleim
S.S. Fine	S.J. Roselle
A.B. Gilliland (organizer/co-chair)	D.B. Schwede
S.C. Howard	A.R. Torian
S.K. LeDuc	J.O. Young

International Symposium on Measurement of Toxic and Related Air Pollutants, Research  
Triangle Park, NC, September 12–14, 2000.

O.R. Bullock, Jr.	S.G. Perry
J.K.S. Ching	W.B. Petersen
B.K. Eder	T.E. Pierce
B.W. Gay	J.E. Pleim
W.T. Hutzell	S.J. Roselle
S.K. LeDuc	K.L. Schere
M.R. Meburst	J.L. West
T.L. Otte	

Hyperspectral Imagery and Water Quality Workshop, Raleigh, NC, September 15, 2000.

A.B. Gilliland

## APPENDIX E: VISITING SCIENTISTS

1. Dr. Deborah H. Bennett  
Lawrence Berkeley National laboratory  
Cyclotron Road, MS-903058  
Berkeley, CA 94720

Dr. Bennett visited FMF on June 20, 2000, for the day to discuss potential collaboration on pesticide spray drift modeling.

2. Mr. Alan Cimorelli  
EPA Region 3  
Philadelphia, PA

Mr. Cimorelli visited FMF from March 6 to March 10, 2000, to collaborate on AERMOD development project.

3. Dr. Thomas E. Gill  
Wind Science & Engineering  
Department of Civil Engineering  
Texas Tech University  
Lubbock, TX

Dr. Gill visited FMF from May 31 to June 2, 2000, to discuss the collaborative project on aerosol chemistry.

4. Dr. Sven-Erik Gryning  
Riso National Laboratory  
Roskilde, Denmark

Dr. Sven-Erik Gryning visited the Division on November 17 and 18, 1999, to aid the Division Director in the final selection of papers and posters to be presented at the Millennium (24th) NATO/CCMS International Technical Meeting on Air Pollution Modeling and Its Application to be held in Boulder, CO, during May 2000.

5. Dr. Shan He  
University of Iowa  
Civil and Environmental Department  
Center for Global and Regional Environmental Research  
Iowa City, IA

Dr. Shan He visited the Division on July 20, 2000, to present a seminar on *The impact of tropospheric aerosol-radiation interaction on photochemical oxidant cycle and climate forcing*.

6. Dr. Gabriel Katul  
School of the Environment  
Duke University  
Durham, NC

Dr. Katul and six students visited FMF on March 29, 2000, as part of the Environmental Engineering 356 class to observe experiments in the wind tunnels and convection tank.

- 7.. Dr. Avi Lacser  
Israel Institute for Biological Research  
Ness Ziona  
Israel

Dr. Avi Lacser arrived on October 25, 1999, to work for approximately two years with AMDB on neighborhood scale modeling.

8. Mr. Chris Leigh  
Mr. David Mottershead  
Dr. Trudie McMullen  
UK Department of the Environment  
National Air Quality Strategies Group  
London, England

Mr. Chris Leigh, Mr. David Mottershead, and Dr. Trudie McMullen visited the Division on November 19, 1999, to discuss Division modeling activities.

9. Rokjin Park  
Department of Meteorology  
University of Maryland  
College Park, MD

Mr. Park visited the Division on July 20 and 21, 2000, to coordinate work on the CMAQ photolysis rate model.

10. Dr. S.T. Rao  
New York Department of Environmental Conservation  
Albany, NY

Dr. Prasad Kasibhatla  
Duke University  
Durham, NC

Dr. S.T. Rao and Dr. Prasad Kasibhatla visited the Division on February 10, 2000, to present a seminar entitled *An intercomparison study of two regional-scale photochemical modeling systems*.

11. Dr. Qingyun Song  
Atmospheric Environment Service  
Ontario, Canada

Dr. Song visited the Division from February 27 to March 10, 2000, to test a new resolved cloud model in CMAQ.

12. Dr. Seiji Sugata  
Takezono 1-803-506  
Tsukuba, Ibaraki, 305-0032  
Japan

Dr. Seiji Sugata visited the Division from May 22 to 26, 2000, to discuss Models-3/CMAQ.

13. Dr. Jay Turner, and Mr. Brian Long  
Department of Environmental Policy  
Washington University  
St. Louis, MO

Dr. Turner and Mr. Long visited the Division on February 25, 2000, to discuss research findings from the OZark Isoprene Experiment (OZIE).

14. Dr. Jeffery Weil  
CIRES  
Boulder, CO

Dr. Weil visited FMF on March 2 and 3, 2000, to collaborate on an internal grant project on convective boundary layer.

## **APPENDIX F: HIGH SCHOOL, UNDERGRADUATE, AND GRADUATE STUDENTS, AND POSTDOCTORAL RESEARCHERS**

1. Dr. Jeffrey R. Arnold  
University Corporation for Atmospheric Research  
Boulder, Colorado

Dr. Arnold, a postdoctoral researcher, is in his third year with the Division. Dr. Arnold is developing more advanced methods to extend the state of the art of diagnostic model evaluation applicable to complex, nonlinear photochemical models, to codify the new evaluation techniques, and to make weight-of-evidence approaches objective.

2. Rokjin Park  
Department of Meteorology  
University of Maryland  
College Park, MD

Mr. Park, a graduate student, is working with the Division to develop a method for adjusting photolysis rates for the presence of aerosols.

3. Dr. Shan He  
University Corporation for Atmospheric Research  
Boulder, CO

Dr. He, a post-doctoral researcher, is working with the Division on air quality model evaluation for particulate matter. He began a 2-year visit with the Division on August 21, 2000.

4. Mr. Jason Smith  
University of North Carolina at Chapel Hill  
Chapel Hill, NC

Mr. Smith, a research assistant funded through UCAR, assisted in the software framework design of the Multimedia Integrated Modeling System (MIMS).

5. Dr. Gail S. Tonnesen  
University Corporation for Atmospheric Research  
Boulder, Colorado

Dr. Tonnesen, a postdoctoral researcher, completed her third year with the Division. Dr. Tonnesen investigated the identification of indicator ratios of ambient concentrations of photochemically active trace gases that might distinguish the sensitivity of the local production of ozone to  $\text{NO}_x$  and VOC emissions in the ambient atmosphere for the testing of air quality models. The tests were developed from theoretical considerations of atmospheric photochemistry.

## **APPENDIX G: ATMOSPHERIC SCIENCES MODELING DIVISION STAFF AND AWARDS**

All personnel are assigned to the U.S. Environmental Protection Agency from the National Oceanic and Atmospheric Administration, except those designated EPA, who are employees of the EPA; PHS, who are members of the Public Health Service Commissioned Corps, or SEEP, who are part of the Senior Environmental Employment Program.

### **Office of the Director**

Francis A. Schiermeier, Supervisory Meteorologist, Director  
Herbert J. Viebrock, Meteorologist, Assistant to the Director  
Dr. Robin L. Dennis, Physical Scientist  
Dr. Basil Dimitriadis (EPA), Physical Scientist (Until June 2000)  
Dr. Peter L. Finkelstein, Physical Scientist  
Bruce W. Gay, Jr. (EPA), Program Manager  
Evelyn M. Poole-Kober, Librarian  
Jeffrey L. West, Physical Science Administrator (Since May 2000)  
Barbara R. Hinton (EPA), Secretary

### **Atmospheric Model Development Branch**

Kenneth L. Schere, Supervisory Meteorologist, Chief  
Dr. Francis S. Binkowski, Meteorologist  
O. Russell Bullock, Jr., Meteorologist  
Dr. Daewon W. Byun, Physical Scientist  
Dr. Jason K.S. Ching, Meteorologist  
Dr. Brian K. Eder, Meteorologist  
Gerald L. Gipson (EPA), Physical Scientist  
James M. Godowitch, Meteorologist  
Dr. William T. Hutzell (EPA), Physical Scientist  
Dr. Michelle R. Mebust (EPA), Physical Scientist  
Tanya L. Otte, Meteorologist  
Dr. Jonathan E. Pleim, Physical Scientist  
Shawn J. Roselle, Meteorologist  
Tanya L. McDuffie, Secretary



## **Modeling Systems Analysis Branch**

Joan H. Novak, Supervisory Computer Specialist, Chief (Until September 2000)  
Dr. William G. Benjey, Physical Scientist  
Dr. Steven S. Fine, Computer Specialist (Since June 2000)  
Dr. Alice B. Gilliland, Physical Science Administrator  
Steven C. Howard, Computer Specialist  
Dr. Sharon K. LeDuc, Physical Scientist  
Thomas E. Pierce, Meteorologist  
John H. Rudisill, III, Equipment Specialist  
Alfreida R. Torian, Computer Specialist  
Gary L. Walter, Computer Scientist  
Dr. Jeffrey O. Young, Mathematician  
Carol C. Paramore, Secretary (Until September 2000)

## **Applied Modeling Research Branch**

William B. Petersen, Supervisory Physical Scientist, Chief  
Dr. Ellen J. Cooter, Meteorologist  
Dr. Dale A. Gillette, Physical Scientist  
Dr. Alan H. Huber, Physical Scientist  
Robert E. Lawson, Jr., Physical Scientist (Until September 2000)  
Dr. Steven G. Perry, Meteorologist  
Donna B. Schwede, Physical Scientist  
John J. Streicher, Physical Scientist  
CDR. Roger S. Thompson (PHS), Environmental Engineer (Until July 2000)  
Lawrence E. Truppi, Meteorologist  
Jonathan Petters (EPA), Engineering Technician (Summer)  
Ashok Patel (SEEP), Engineer  
John Rose (SEEP), Machinist/Model Maker  
Bruce Pagnani (SEEP), Computer Programmer  
Sherry A. Brown, Secretary

## **Air Policy Support Branch**

Mark L. Evangelista, Supervisory Meteorologist, Chief  
Dennis A. Atkinson, Meteorologist  
Dr. Desmond T. Bailey, Meteorologist  
Patrick D. Dolwick, Physical Scientist  
John S. Irwin, Meteorologist  
Brian L. Orndorff, Meteorologist  
Norman C. Possiel, Jr., Meteorologist  
Jawad S. Touma, Meteorologist

## **FY-2000 AWARD**

Air Resources Laboratory Paper of the Year Award - 1999, awarded in October 2000.

Byun, D.W. Dynamically consistent formulations in meteorological and air quality models for multiscale atmospheric studies. Part I: Governing equations in a generalized coordinate system. *Journal of the Atmospheric Sciences* 56:3789–3807 (1999).

Byun, D.W. Dynamically consistent formulations in meteorological and air quality models for multiscale atmospheric studies. Part II: Mass conservation issues. *Journal of the Atmospheric Sciences* 56:3808–3820 (1999).